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Monte Carlo Simulations of Suprathermal Enhancement in Advanced Nuclear Fusion Fuels

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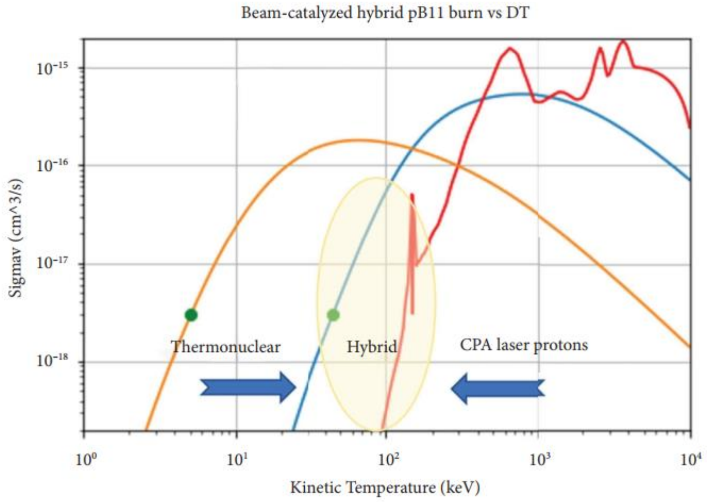
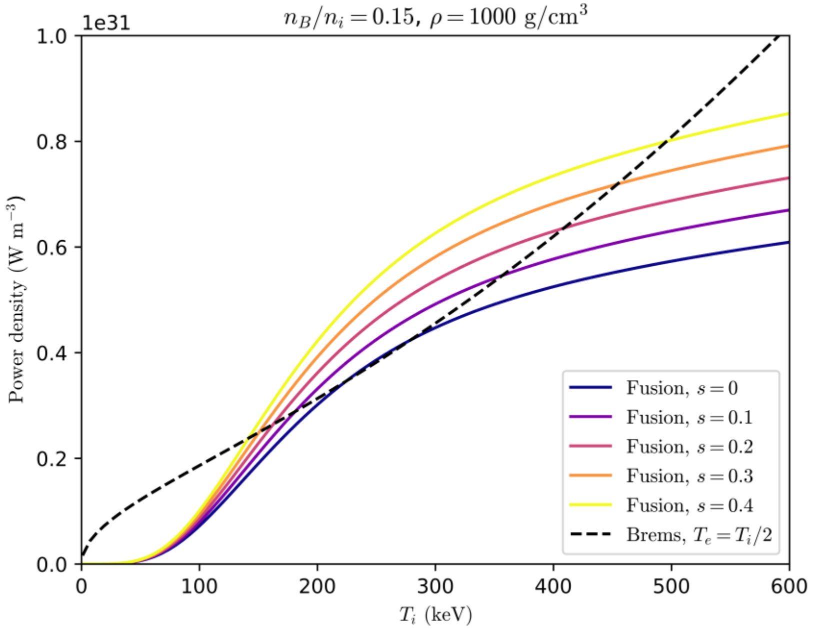
Why Suprathermal Effects Matter?

- Fusion products and fast ignitor protons will slow in the bulk plasma and create non-thermal energy distributions [1].
- Up-scattering of thermal protons/injection of fast protons will increase fuel reactivity.
- Suprathermal enhancement increases the burn window where fusion power > brems losses.
- **Enhancement is critical for self-heating and burn propagation.**
- Small-angle Fokker-Planck simulations [2] suggest 10-20% effect in MCF plasmas – enhancement at ICF conditions unknown.
- Current models crudely approximate suprathermal effects using a constant reactivity multiplier.

$$P_{fus} = (1+s)Qn_1n_2\langle\sigma v\rangle V$$



Fusion reactivity for thermonuclear pB11 and DT, and beam-driven pB11. [1]



Burn window for different suprathermal enhancements. [3,4]

[1] Mehlhorn *et al.*, Laser and Particle Beams, 2022
[2] Putvinski, Ryutov & Yushmanov, Nuclear Fusion, 2019
[3] Svensson, Astrophysical Journal, 1982
[4] Tentori & Belloni, Nuclear Fusion, 2023

Evidence of Suprathermal Effects on NIF

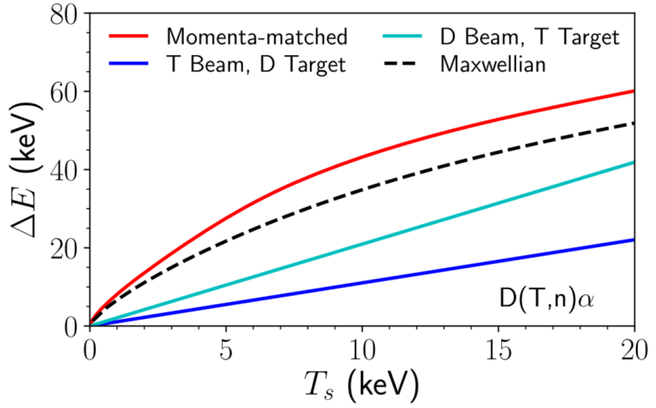
- Shape of particle distribution inferred from neutron spectral analysis. For DT:

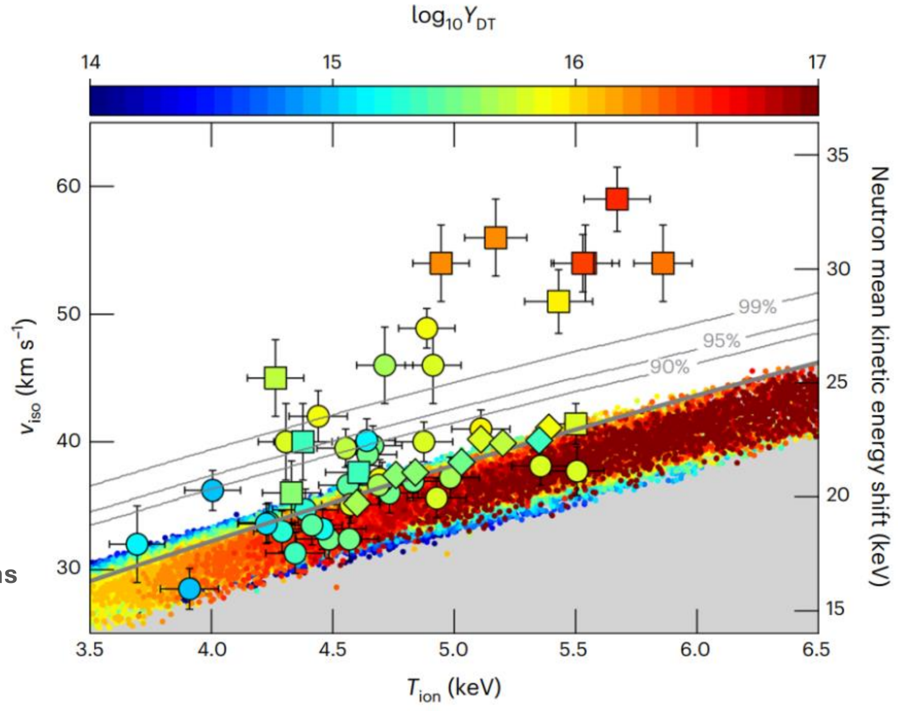
$$\Delta E_n = \frac{4}{5}\langle K_{rel}\rangle + \frac{1}{2}m_p\langle v_{CM}^2\rangle, \quad T_i = \frac{5}{3}m_p\langle v_{CM}^2\rangle$$

  Where a Maxwellian distribution corresponds to the 'hydrodynamic boundary'

- Departure from hydrodynamic boundary indicative of more 'momentum-matched' collisions [9] – high relative velocity, low CM velocity
- NIF burning plasma experiments [5] have observed increased neutron yield and greater neutron upshift compared to HYDRA simulations.
  - Other PIC simulations [6] have also not predicted this effect. Most are based on the Takizuka & Abe [7] (Gaussian central limit) or Nanbu [8] (cumulative small-angle) treatment of Coulomb scattering.

Limiting cases for neutron spectral analysis for isotropic distributions. [9]



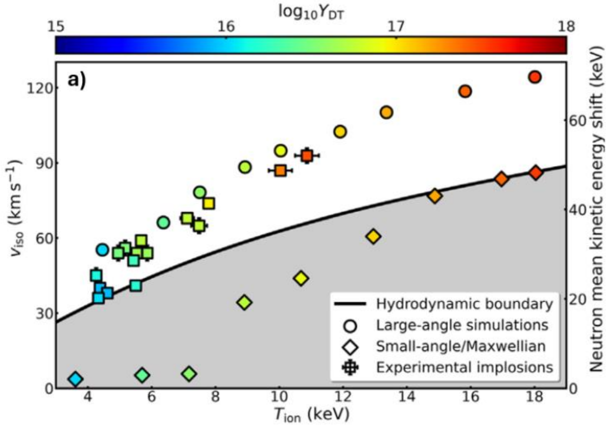


Neutron spectral analysis of NIF experiments and HYDRA simulations (2D and 3D). Squares are burning plasma shots. [9]

[5] Hartouni *et al.*, Nature Physics, 2022
[6] Sherlock & Rose, High Energy Density Physics, 2009
[7] Takizuka & Abe, Journal of Computational Physics, 1977
[8] Nanbu, Physical Review E, 1997
[9] Crilly *et al.* Nuclear Fusion, 2022

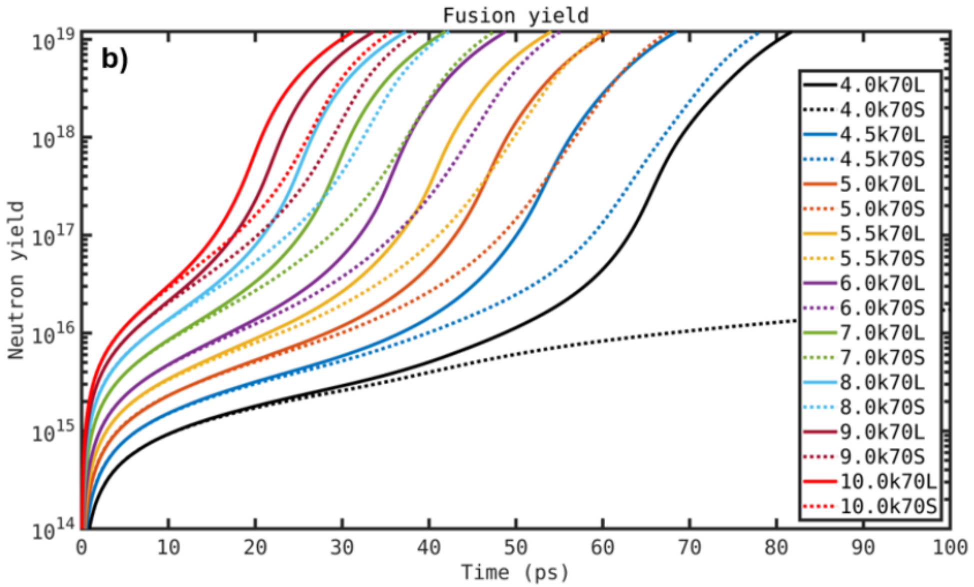
Large-Angle Collisions

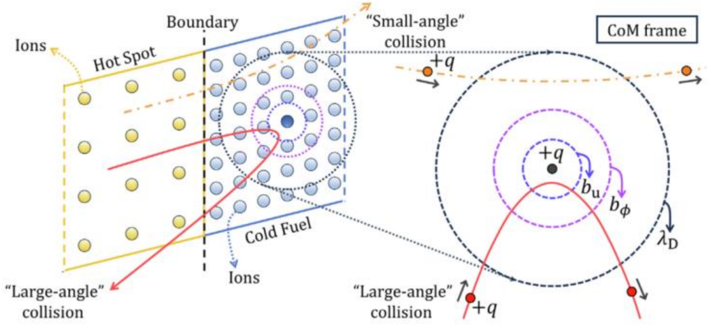
- The LAPINS PIC code has been recently modified to include large-angle collisions [10]
  - Large-angle collisions facilitate larger energy transfer, which 'lifts' the fuel ion distribution tail as alphas slow down
  - The highly nonlinear fusion cross section favours head-on (e.g. momentum-matched) collisions in this tail
- Departure from small-angle and large-angle kinetic results occurs at onset of burn-propagation - more rapid alpha deposition at the hotspot boundary expedites hotspot expansion and leads to 'cooler' burning
- Cutoff determined when potential from target greater than superposition potential from all other field species [11]



Neutron spectral analysis of LAPINS simulations plotted alongside NIF data [10]

Fusion yield for LAPINS simulations w/ and w/o large-angle scattering [10]





$$\frac{e^{-b_\phi/\lambda_{De}}}{b_\phi/\lambda_{De}} = \sum_{m=1}^{\infty} \frac{e^{-m^{1/3}x}}{m^{1/3}x}, \qquad x = \frac{1}{\lambda_{De}}\left(\frac{3}{4\pi n_s}\right)^{1/3}$$

$$b_c = \sqrt{b_\phi(b_\phi - 2b_\perp)}$$

Ion trajectories for small and large-angle collisions [11]

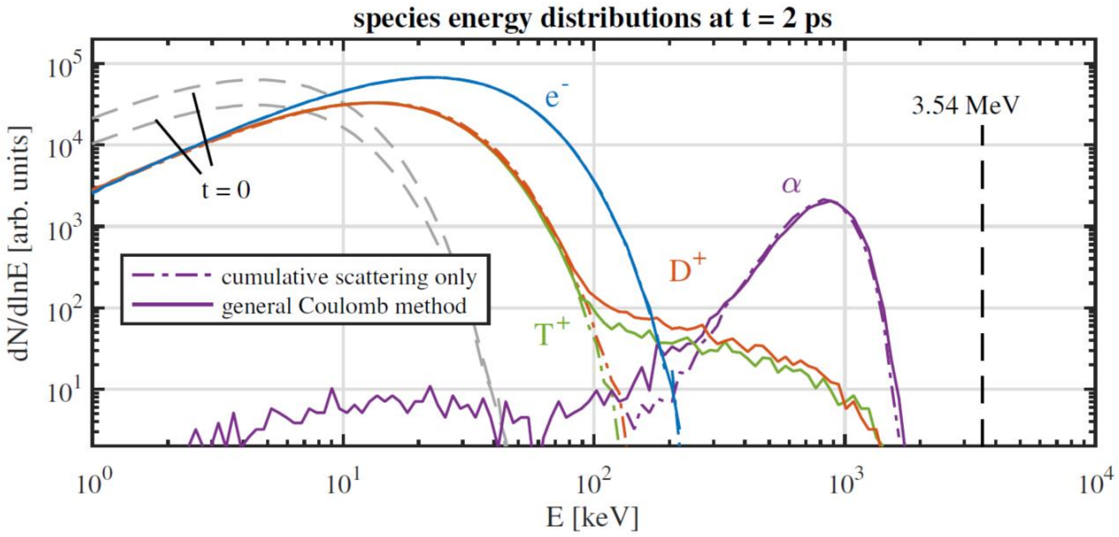
[10] Xue, Wu & Zhang, Science Bulletin, 2025
[11] Turrell, Sherlock & Rose, Journal of Computational Physics, 2015

Large-Angle Collisions

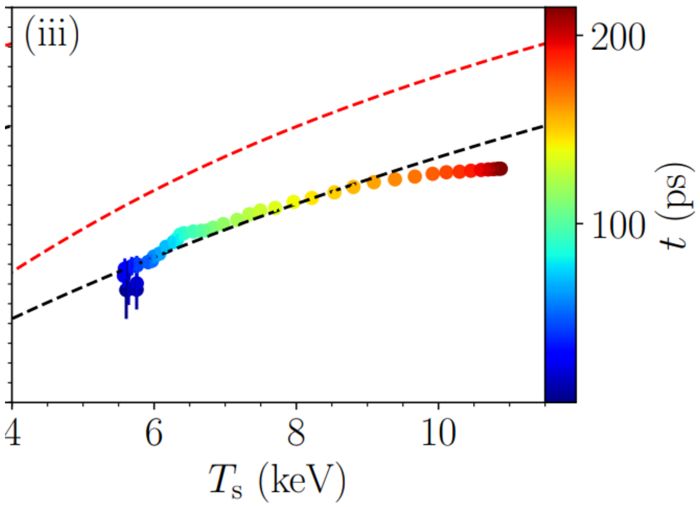
- LLNL have also started to investigate suprathermal effects with the PICNIC code [12, 13]
  - Cumulative Coulomb + large-angle Rutherford + α-D, α-T, D-T nuclear elastic scattering + anisotropic fusion
  - Coulomb sampling accounts for electron screening and quantum diffraction

$$\sin^2\frac{\theta}{2} = \frac{b_\perp^2 + b_{\mathrm{qm}}^2}{b_\perp^2 + \left(b + b_{\mathrm{qm}}\right)^2}$$

- Unlike the NIF results or LAPINS, PICNIC has not observed any suprathermal enhancement
  - LAPINS samples **both** the small and large angle scatter, and adds them together
  - PICNIC samples **either** the small or large angle scatter, but truncates the large angle collision probability at 10%



Alpha slowing down in DT using the PICNIC code [12]



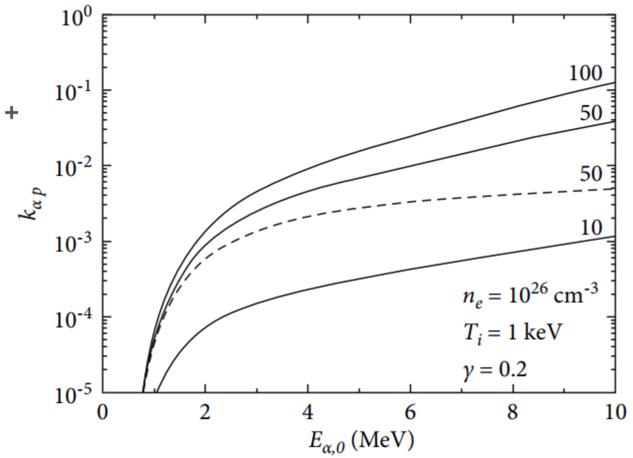
Neutron spectral analysis of PICNIC simulations of the N210808 NIF shot [13]

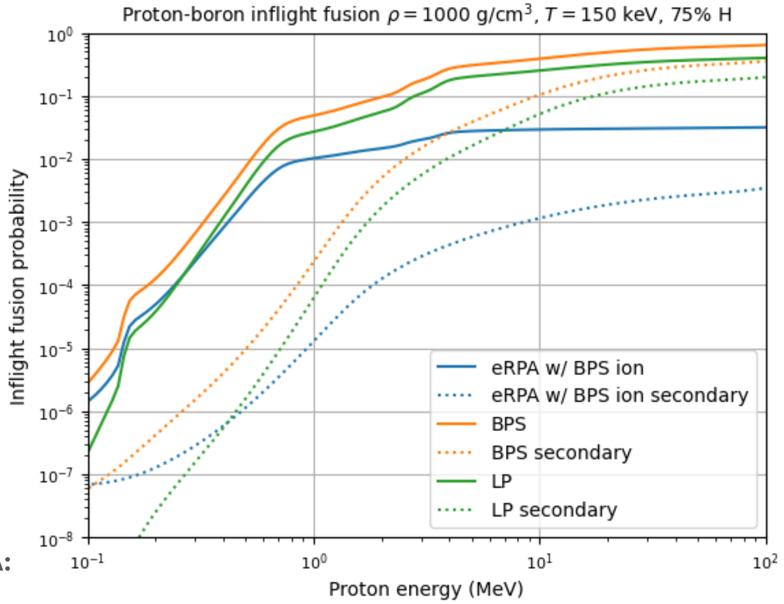
[12] Angus & van de Wetering, Journal of Computational Physics, 2025
[13] Van de Wetering *et al.* arXiv, 2025

Multiplication Processes in pB11

- Belyaev *et al.* [14] hypothesized that a chain reaction could occur via $^{11}B(\alpha,p)^{14}C$, but this is suppressed when ionic and electronic stopping is considered [15]
- Eliezer *et al.* [16] proposed the α-p 'avalanche' to explain high yield shots on PALS, but the timescale to develop is longer than the TOF signal time [17]
- Belloni [18] has investigated the effects of α-p up-scattering in hot-electron pB11 to determine enhancement for cold fuel heating
  - Nuclear elastic scattering has been included
  - Increasing the multiplication factor above 1% is problematic, α-p up-scattering unlikely to make a difference at least for cold fuels
- Proton fast ignition can be particularly effective at heating pB11 due to inflight fusion and p-p up-scattering
  - 20-40% fusion probability for 10 MeV protons @ 150 keV, 1000 g/cc, including secondary fusions

α-p multiplication in cold pB11 [4]. Dashed line is scattering without nuclear + interference corrections.





Proton inflight fusion probability with p-p secondaries included. Strong dependence on stopping power model - LP: Li-Petrasso [19], eRPA: enhanced RPA, BPS: Brown-Preston-Singleton

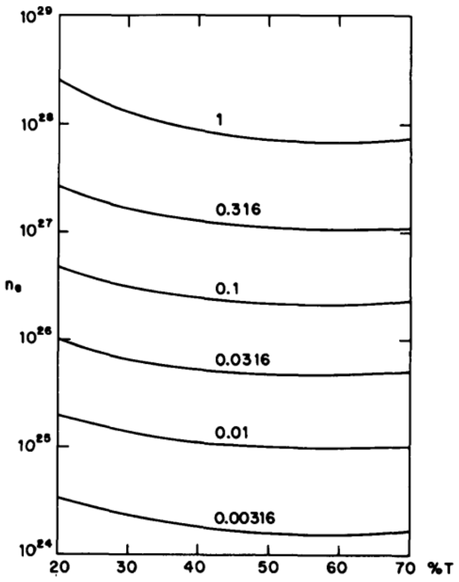
[14] Belyaev *et al.*, Laser Physics Letters, 2015
[15] Shmatov, Physics of Atomic Nuclei, 2016
[16] Eliezer *et al.*, Physics of Plasmas, 2016
[17] Belloni *et al.*, Physics of Plasmas, 2018
[18] Belloni, Lasers and Particle Beams, 2022
[19] Zylstra *et al.*, Physics of Plasmas, 2019

Chain reactions with neutrons – a saving grace?

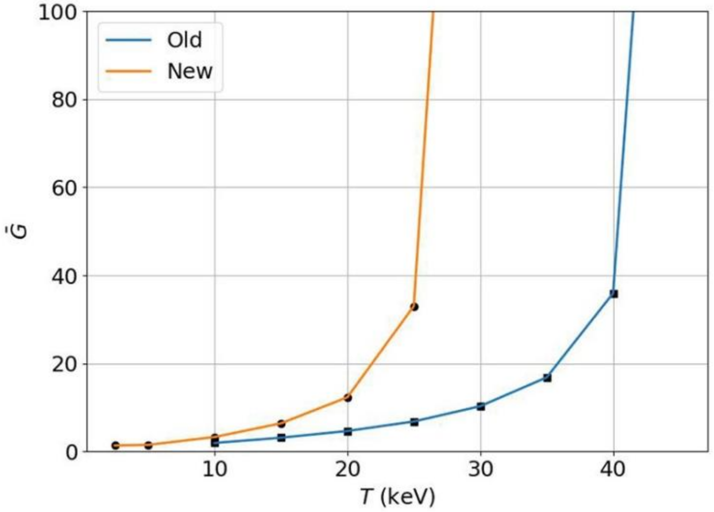
- Robinson published two papers on DD chain reactions in 2024, one for non-degenerate [20] and one for degenerate [21] plasmas, plus a correction to the stopping model
  - 0D Monte Carlo model that tracks neutrons, deuterons, protons, tritons and helions in an infinite, homogenous plasma
  - All D-cycle fusion reactions, D(p,n)2p, p-D elastic scattering and neutron-ion elastic scattering considered, taken from ENDF/B-VIII.0 library
  - Ions are slowed down by field ions and electrons each timestep, typical Fokker-Planck approach to stopping model [19]

$$s \approx \frac{Q_{tot} + K_{dep}}{K_{i,0}}$$

- Criticality observed for 6 MeV deuterons in DD @ 27 keV, n_i = 1e33 /m^3 and degenerate DD @ n_i = 3.5e33 /m^3
  - Criticality not possible if DT reactions are not included, **neutrons are the dominant mechanism for the chain reaction**
- Peres & Shvarts [21] have shown criticality in degenerate DT @ ni = 8.4e33 /m^3 (using k-eigenvalue approach)



Lines of equal multiplication factor for degenerate DT [22]



Beam gain for 6 MeV deuterons in DD [21]

[20] Robinson, Plasma Physics and Controlled Fusion, March 2024
[21] Robinson, Plasma Physics and Controlled Fusion, October 2024
[22] Peres & Shvarts, Nuclear Fusion, 1975

Research Question and Aims

- Putvinski, Belloni and Robinson have approached studies of suprathermal effects with different methodologies (Fokker-Planck, analytic, Monte Carlo), with different fuels at different regimes. A unified approach is desirable, which addresses

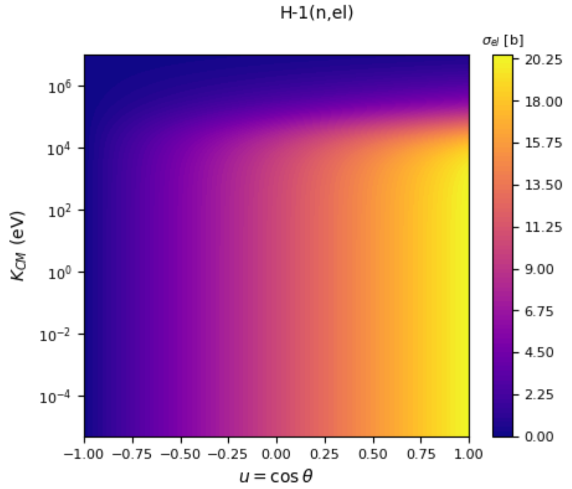
To what extent does burn product transport via large-angle Coulomb scattering, nuclear elastic scattering and nuclear reactions enhance the reactivity of advanced fusion fuels at ICF-relevant conditions?

- Pure pB11 is proving very difficult to burn even with advanced technological capability. A path forward may include mixed fuels with DT or DD seeding, and so

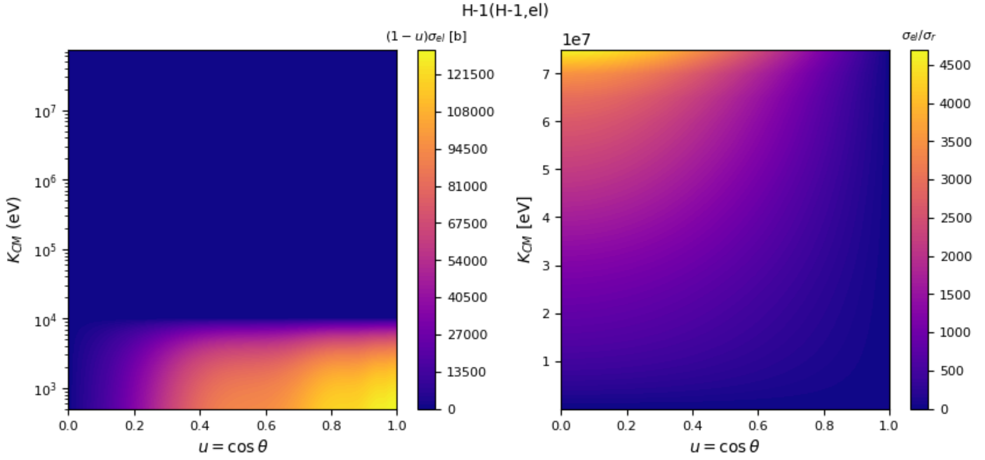
Can fast neutrons drive a critical chain reaction in pB11 if mixed with DT or DD?

Fast Particle Tracker

- We are extending Robinson's method to track the slowing down, up-scattering and fusion of fast n, p, D, T, He-3, α and B-11 in a stationary thermal background plasma
  - Electron collisions and grazing ion collisions are approximated by the Li-Petrasso stopping power [19] instead of simulated directly as in PIC codes
  - The threshold for large-angle ion collisions is determined using the LAPINS screened Coulomb potential cutoff [11], but the angle is sampled using the method from PICNIC
  - Spin-spin coupling and particle indistinguishability have been accounted for in the elastic scattering cross sections
  - All available and relevant neutron and nuclear elastic cross sections in the ENDF database have been included
  - The pB11 alpha spectra is sampled from a first-principles analytic model [23] at the dominant 675 keV resonance
- The focus of this code is the **enable fast parameter scans** of advanced fuels and identify kinetic regimes of interest. Finite boundaries, hydrodynamics and particle transport will reduce the extent of suprathermal enhancement and still require PIC modelling



Cumulative cross-section for p-n scattering



Cumulative cross-section for p-p scattering, and comparison to pure Rutherford scattering

[23] Quebert & Marquez, Nuclear Physics A, 1969

Stopping Power Model

- The Li-Petrasso [19] model is a third-order Fokker-Planck stopping power valid for $\ln \Lambda > 2$ that also includes the effects of electron degeneracy and stopping due to collective plasma oscillations
- The third-order correction (the $\frac{m_i}{m_j}$ terms) are turned off for the ion stopping in favour of MC large-angle sampling
- We note that the original authors have made a mistake in their published derivation and plots, and this has been corroborated with other stopping models

Binary collisions

Stopping on plasmons

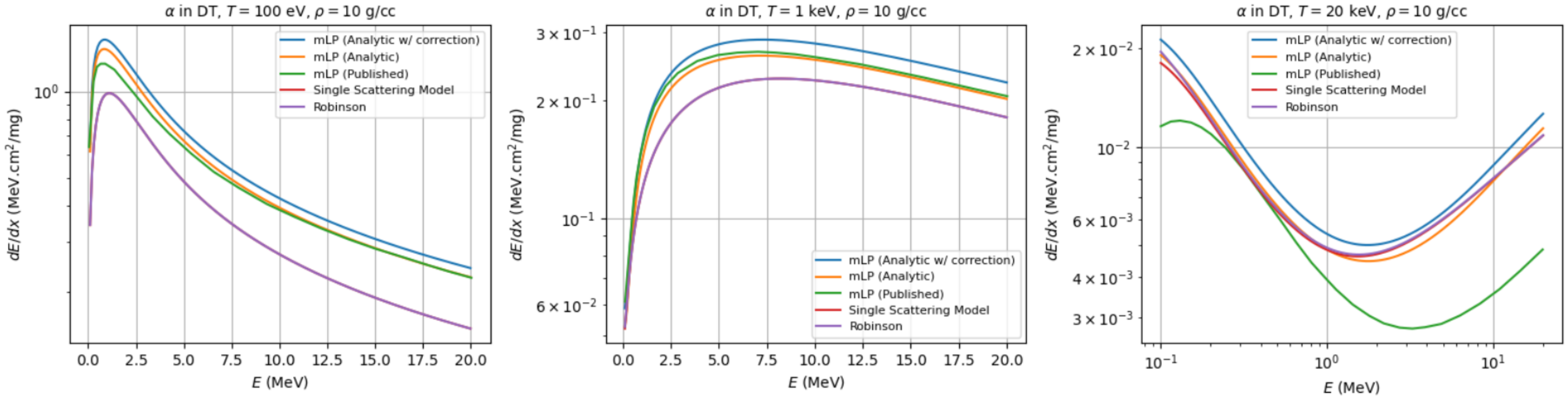
$$\frac{dE_i}{dx} = -\sum_j \frac{4\pi n_j}{m_i}\left(\frac{Z_i Z_j e^2}{4\pi\varepsilon_0 v_i}\right)^2 \left[G(x)\ln\Lambda + \frac{1}{\sqrt{2x}} K_0\left(\frac{1}{\sqrt{2x}}\right) K_1\left(\frac{1}{\sqrt{2x}}\right)\right]$$

$$G(x) = \left(1 + \frac{m_j}{m_i}\frac{1}{\ln\Lambda}\right)\mathrm{Erf}(x) - \left(1 + \frac{m_j}{m_i}\right)\frac{2}{\sqrt{\pi}} x e^{-x^2},$$

where $x = v_i\sqrt{\frac{m_j}{2T_j}}$.

Large-angle Fokker-Planck correction

Comparison of stopping models which strongly suggests publication error



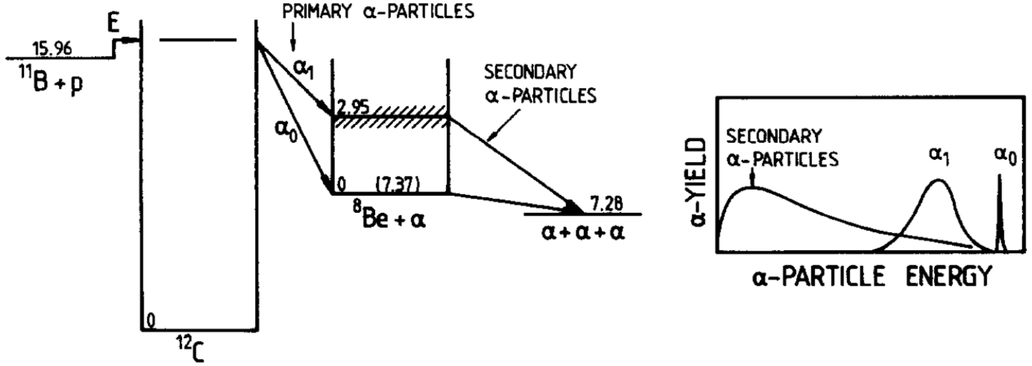
HB11 ENERGY

pB11 Spectra

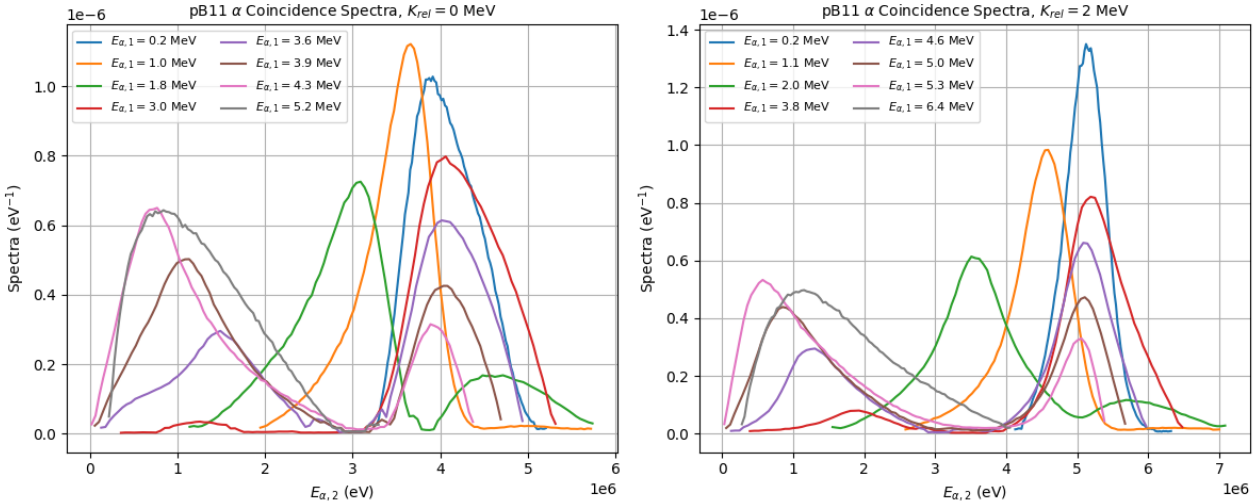
- Quebert and Marquez [23] have provided an analytic form for the pB11 alpha spectra α_1 break-up channel

$$\frac{d^2\sigma}{dE_1 dE_2} \propto |\mathcal{M}|^2$$

- We have tabulated the primary and secondary alpha spectra fir 0-20 MeV collision energies, although under the assumption tof using the 675 keV resonance parameters. Identifying the weightings of each break-up channel as a function of energy would be a welcome addition to the model.

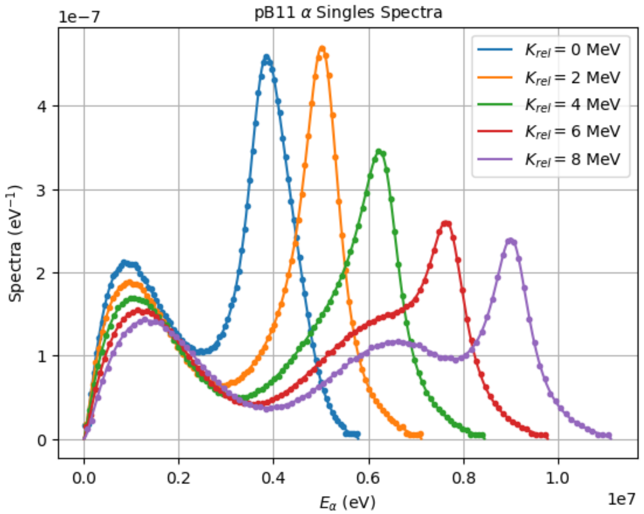


Sequential decay scheme and expected α spectrum for pB11 [24]



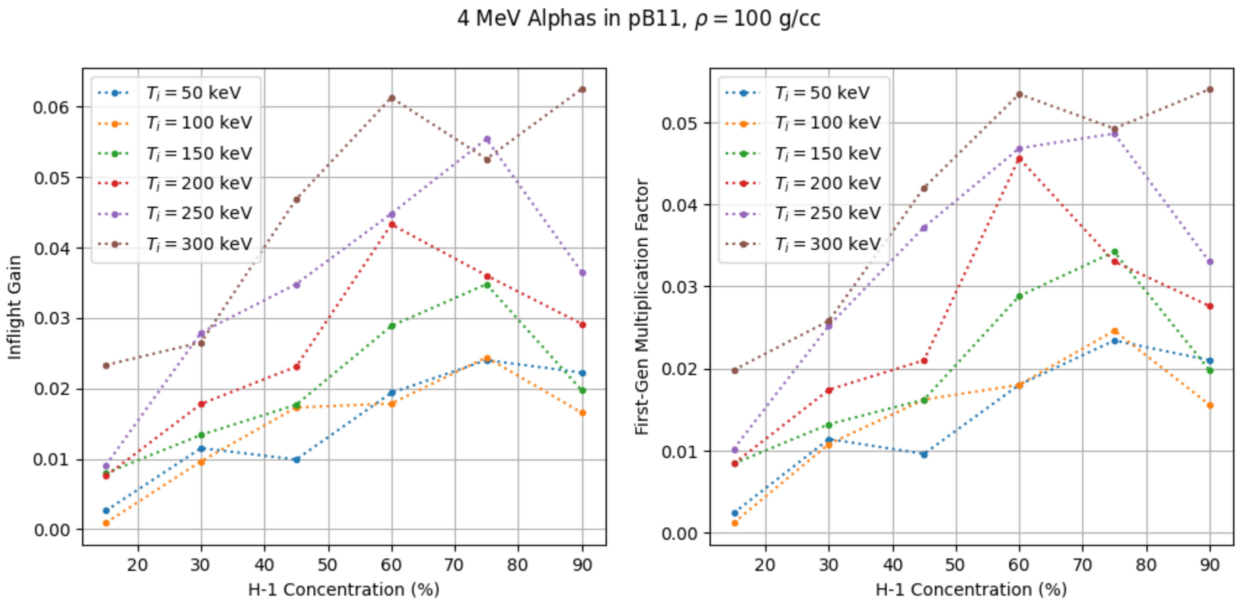
pB11 singles spectra. The dots are the result of Monte Carlo inverse transform sampling, whereas the lines are analytic

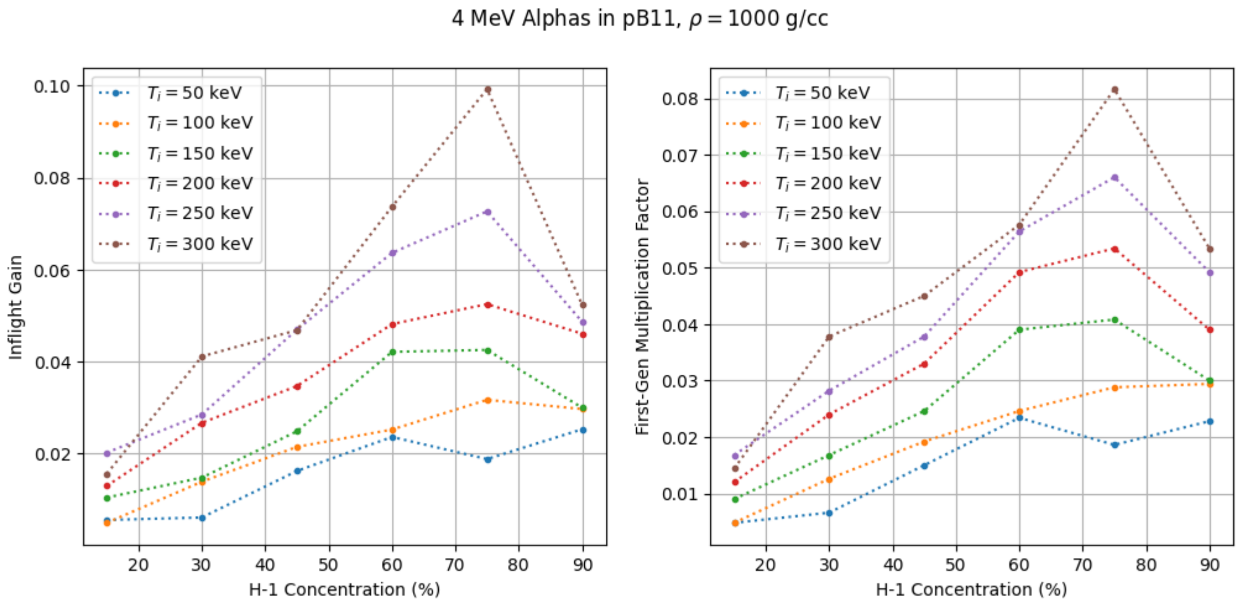
Coincidence spectra at 0 MeV and 2 MeV collision energy



[24] Becker, Rolfs, Trautvetter, Atomic Nuclei, 1987

Results – Pure pB11 Suprathermal Enhancement

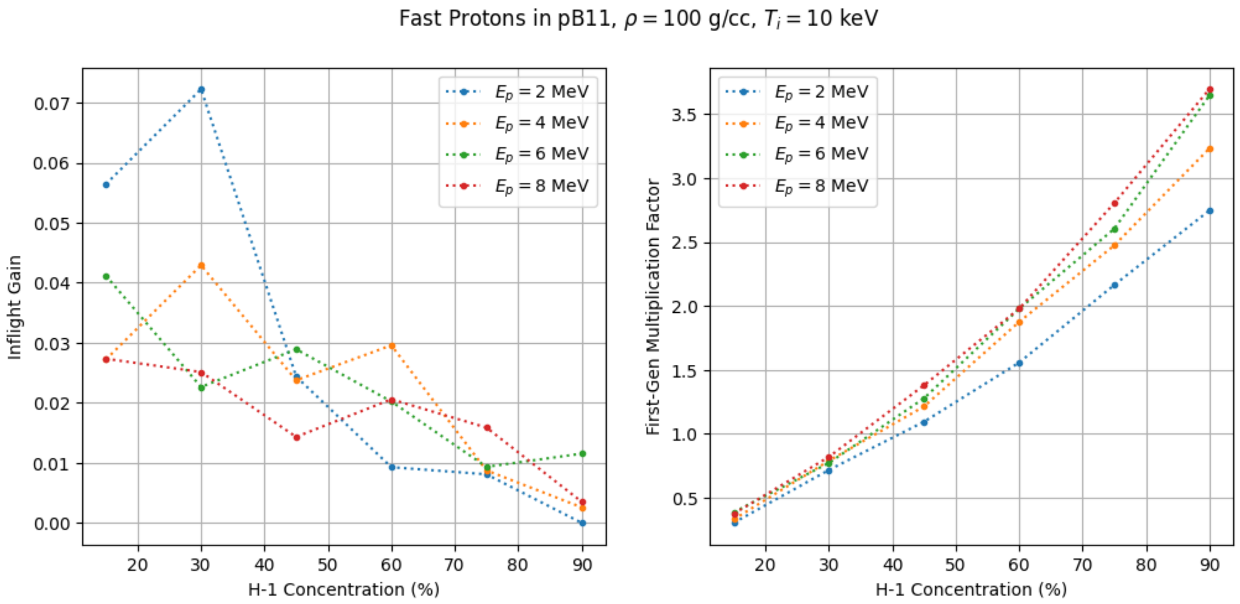


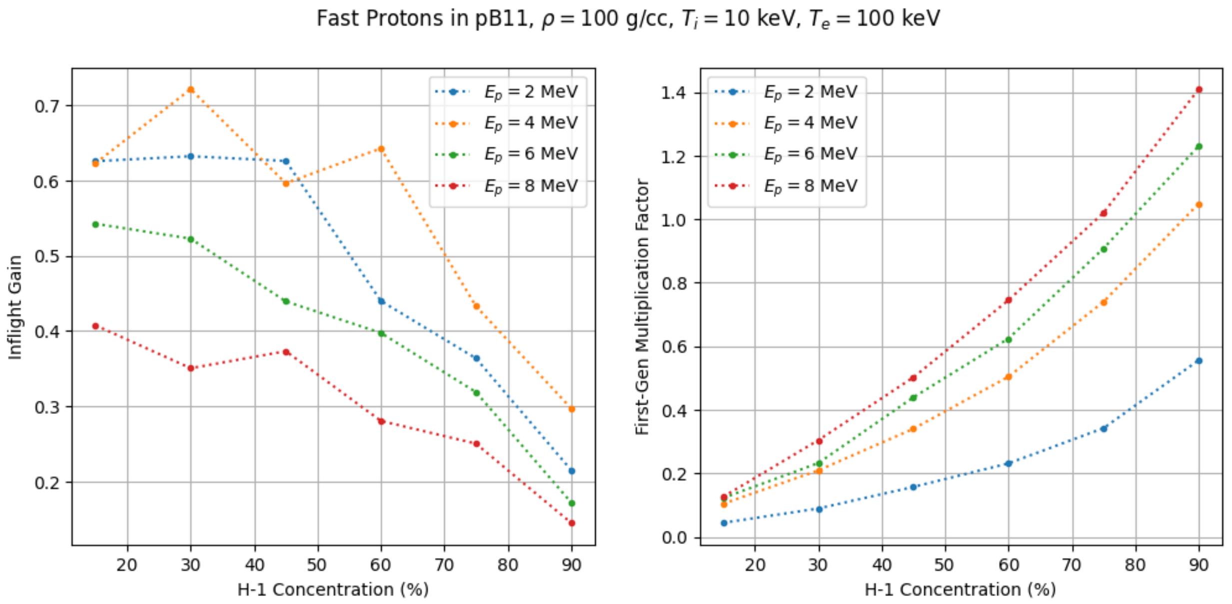


- Contrary to previous modelling assumptions, suprathermal enhancement from α-p up-scattering in pure B-11 contributes no more than 10%, and likely a lot less when transport is considered.
- The prospect of a charged-particle chain reaction in pure pB11 looks highly unlikely for any feasibly achievable plasma regime

$$s \approx \text{Inflight Gain} = \frac{Q_{tot} + K_{dep}}{K_{i,0}}$$

Results – Proton Fast Ignition in pure pB11

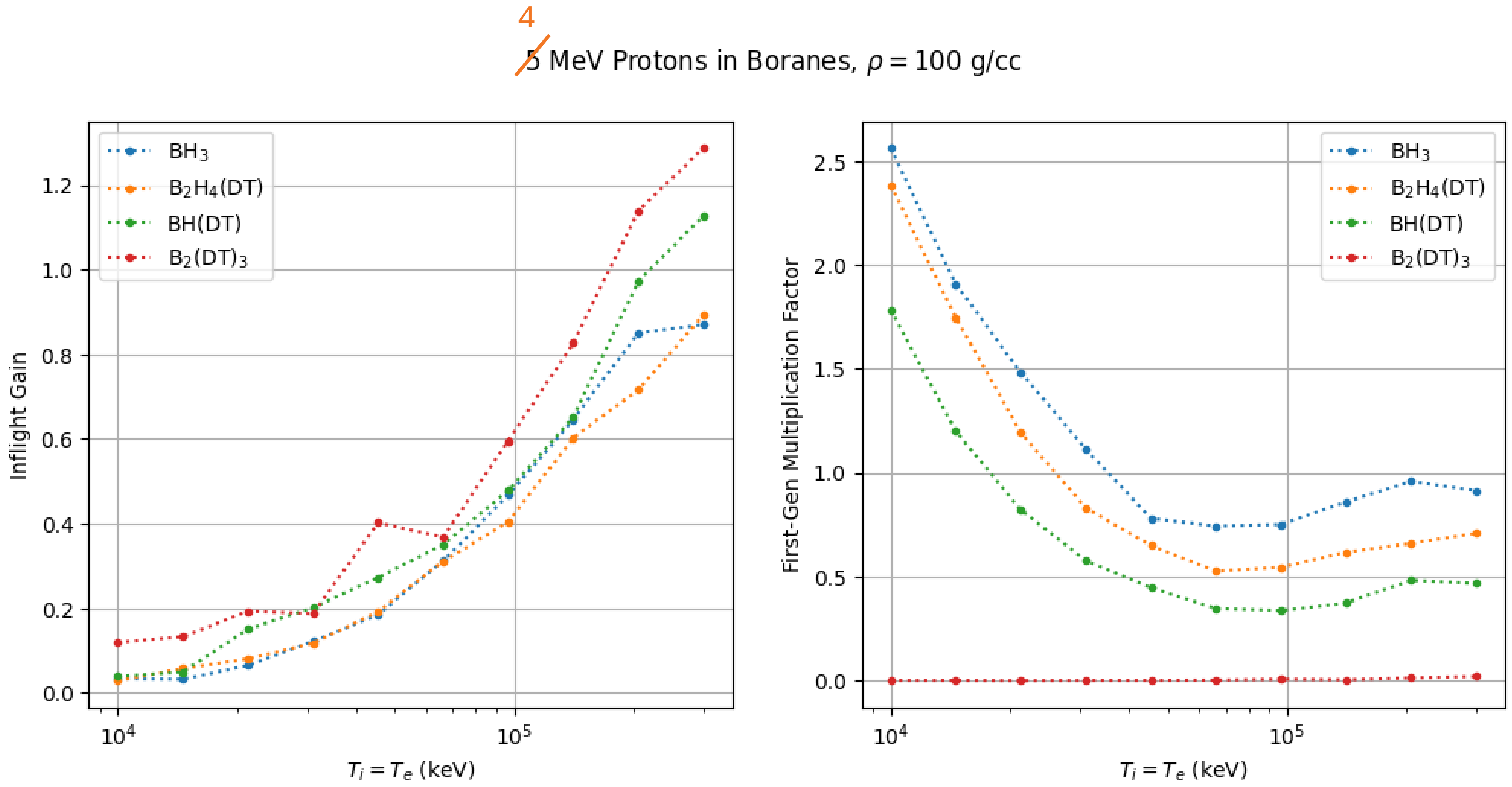




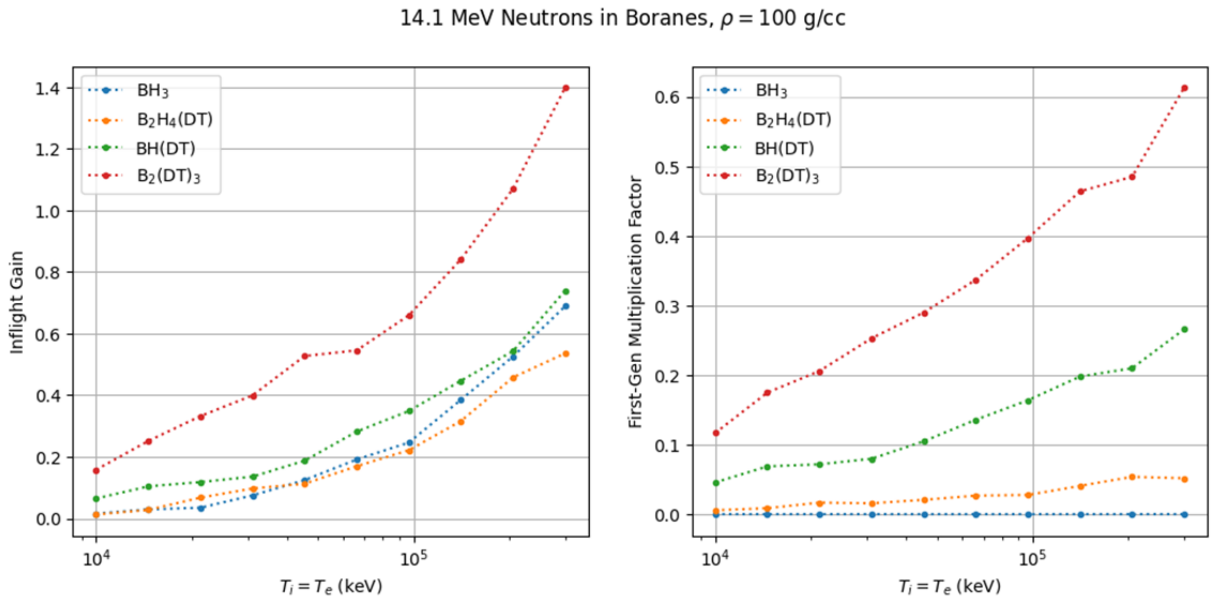
- Fast protons experience more scatter events, but with less average energy transfer, at low temperatures
- Inflight/secondary pB11 fusions only play a significant role in bulk target heating when the plasma is in 'hot electron' mode – 60-70% energy multiplication
- Moreau [25] estimated the multiplication to be 20-30% at these conditions, although this was done with the old cross-section, an outdated stopping power and no consideration of large-angle/NES effects

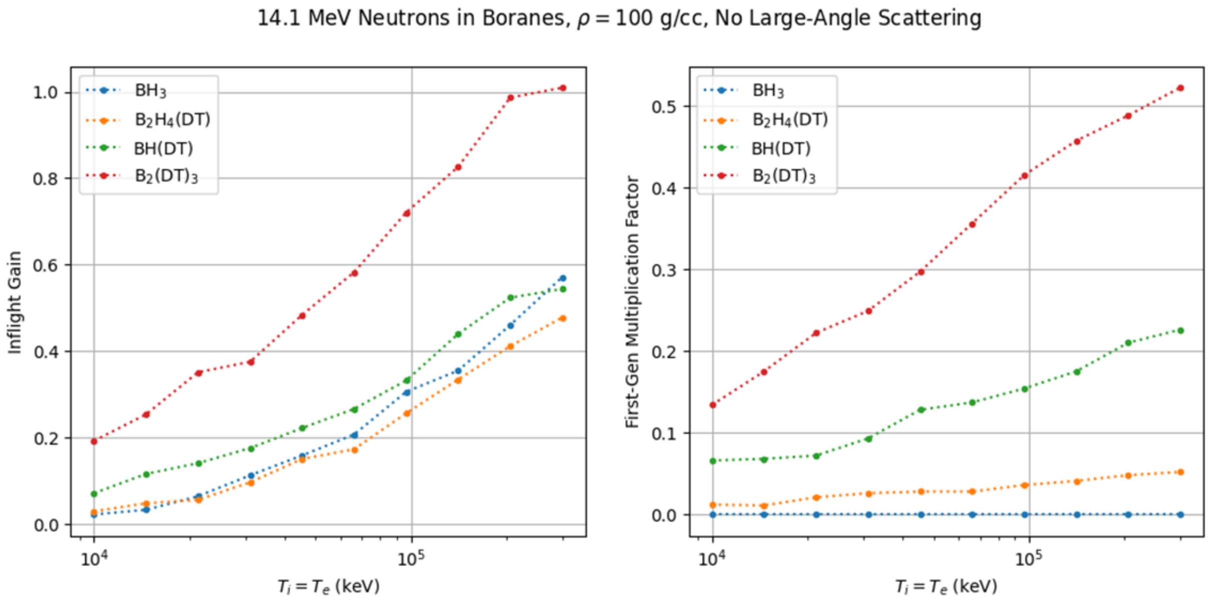
[25] Moreau, Nuclear Fusion, 1977

Results – Proton Fast Ignition in Enriched Boranes



Results – Neutron Multiplication in Enriched Boranes





- Even without the inclusion of large-angle and nuclear elastic scattering, the suprathermal enhancement of mixed DT-pB11 is >20% for Ti > 100 keV
- There is not a huge difference in this enhancement between BH3 and BH(DT) – neutrons couple far better to protons to take advantage of the pB11 cross-section
- Rather than consumed as an aneutronic fuel, the real benefit of boron may be to enable non-cryogenic fuels

The Road Ahead

- This work is still in a preliminary stage and the focus of today was to demonstrate a new capability and new strategy for HB11 and the broader pB11 community – more on Wednesday!
- More extensive parameter sweeps are necessary – different ion/electron temperatures, densities, borohydride chemistries
- Currently exploring the inclusion of Li-6 to take advantage of aneutronic p-Li6 fusion and internal tritium breeding for low tritium targets
- This model can provide suprathermal enhancement factors as a function of fuel conditions, but it is inherently limited as a 0D code
    - Open to exploring 1D models or integrating some of the new collision physics into existing MC/PIC codes

And please see the talks from my colleagues!

Igor Morozov – **9am Wednesday**

Numerical simulations of ignition and fusion burn wave propagation in proton-boron fuel

Anna Ghorbanpour – **11am Wednesday**

Optimising proton-boron-11 fuel for fast ignition inertial fusion applications.