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Towards accurate and efficient mean-field plasma boundary simulations for DEMO with kinetic neutrals

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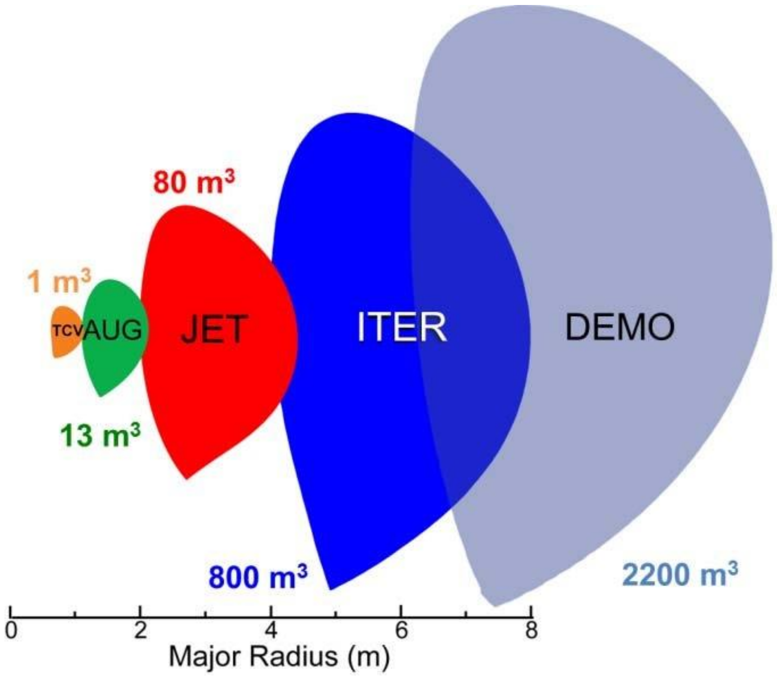
TSVV-5 code camp 21/11/2024

(EU-) DEMO



- At present, conceptual design phase

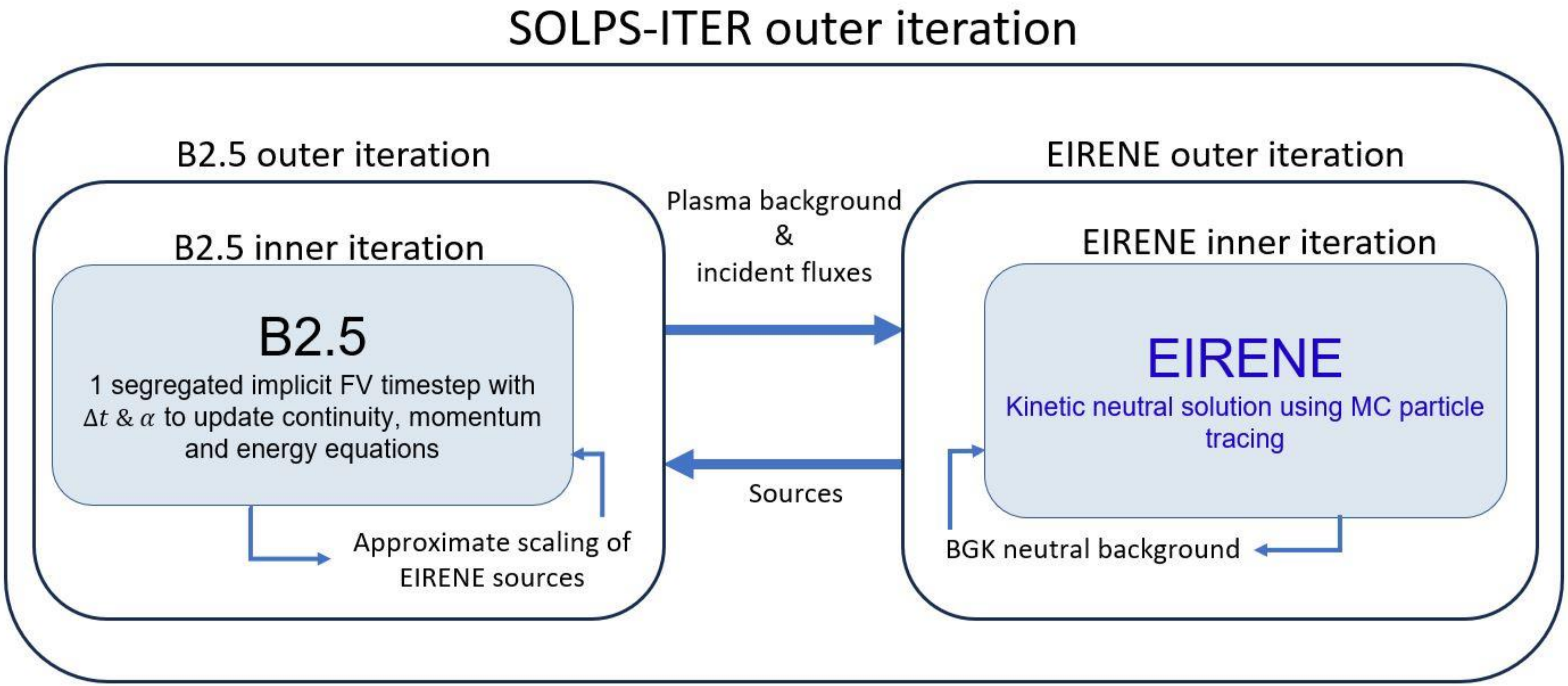
- Need to find possible **operational space**
  2GW fusion plasma ↔ acceptable divertor heat loads and temperatures

→ need for plasma boundary simulations

→ create database of SOLPS-ITER simulations

avoid discovering large numerical errors afterwards

B2.5-EIRENE coupling with fully kinetic neutrals



Random Noise Averaging

- Found to be most efficient coupling strategy in PhD K. Ghoos

- No or limited number of inner B2.5 iterations
- Random seeds (vs. Correlated Sampling)
- No runtime-averaging of source terms (vs. Robbins Monro)
- Run to statistical steady state
- Then start averaging plasma state

Numerical errors in plasma boundary codes

$$\epsilon_{\mathrm{num}} = \epsilon_{\mathrm{d}} + \epsilon_{\mathrm{c}} + \epsilon_{\mathrm{b}} + \epsilon_{\mathrm{s}}$$

ϵ_{s}	statistical error	direct result of noisy MC sources
ϵ_{b}	finite sampling bias error	deterministic error due to noise + non-linearities
ϵ_{c}	convergence error	non-zero residuals
ϵ_{d}	discretization error	finite grid resolution

Error scaling:

- $\epsilon_{\mathrm{s}}: \propto 1/\sqrt{P}$ during run, $\propto 1/\sqrt{P\,I}$ when averaging
- $\epsilon_{\mathrm{bc}} = \epsilon_{\mathrm{c}} + \epsilon_{\mathrm{b}}: \propto \frac{1}{P}$

Towards accurate and efficient DEMO simulations in SOLPS

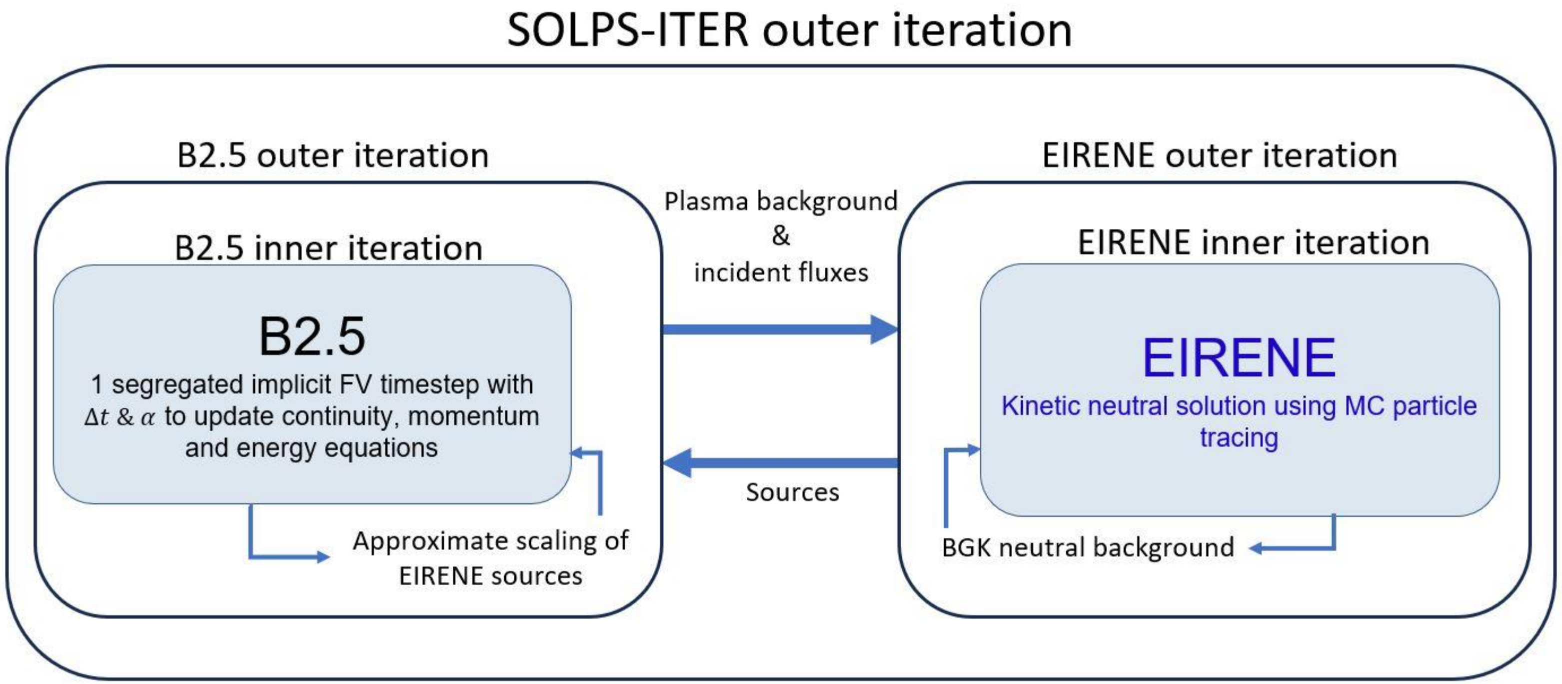
- Goal: acceptable numerical errors for DEMO SOLPS cases (e.g. < 10%) as cheaply as possible

- Start from framework of PhD K. Ghoos

- But, some unanswered questions:
  - Q1: effect of Δt on bias?
  - Q2: effect of NNC on error scaling?
  - Q3: effect of impurities?

Neutral-neutral collisions

- Only plasma-neutral interactions considered in PhD K. Ghoos
- Present-day EIRENE simulations include NNCs
- BGK approximation: collision background is Maxwellian (from previous iteration)



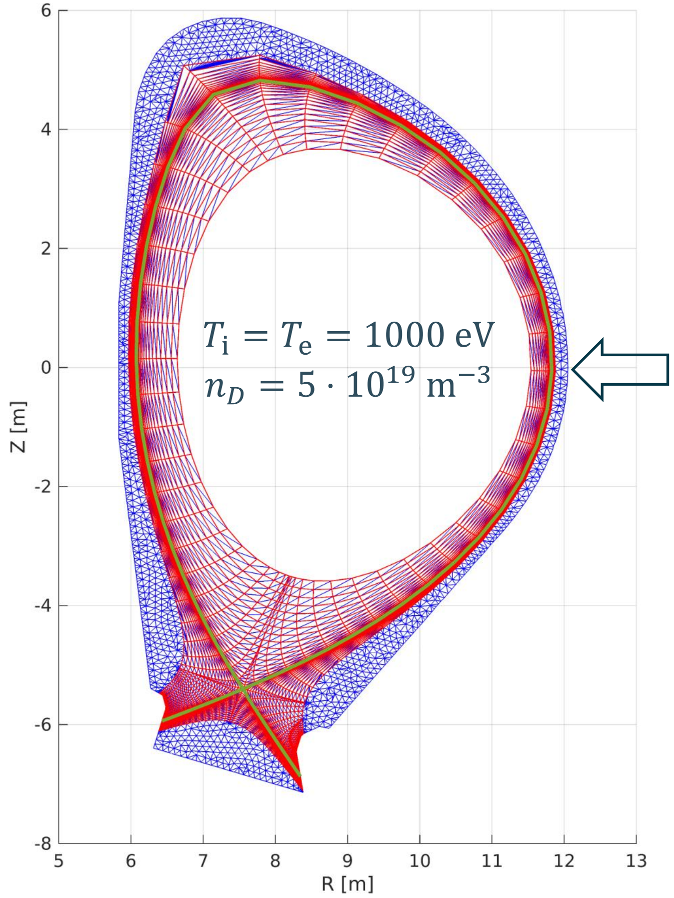
Effect of Δt

- Δt determines how much plasma will adapt to noisy MC sources in 1 iteration
- Small Δt is expected to act as a filter

- *[M. Baeten et al., CtPP, 2018]:* statistical error scales with $\sqrt{\Delta t}$ (0D+1D cases)
- Effect of Δt on bias not studied in PhD K. Ghoos for 2D SOLPS

Case set-ups

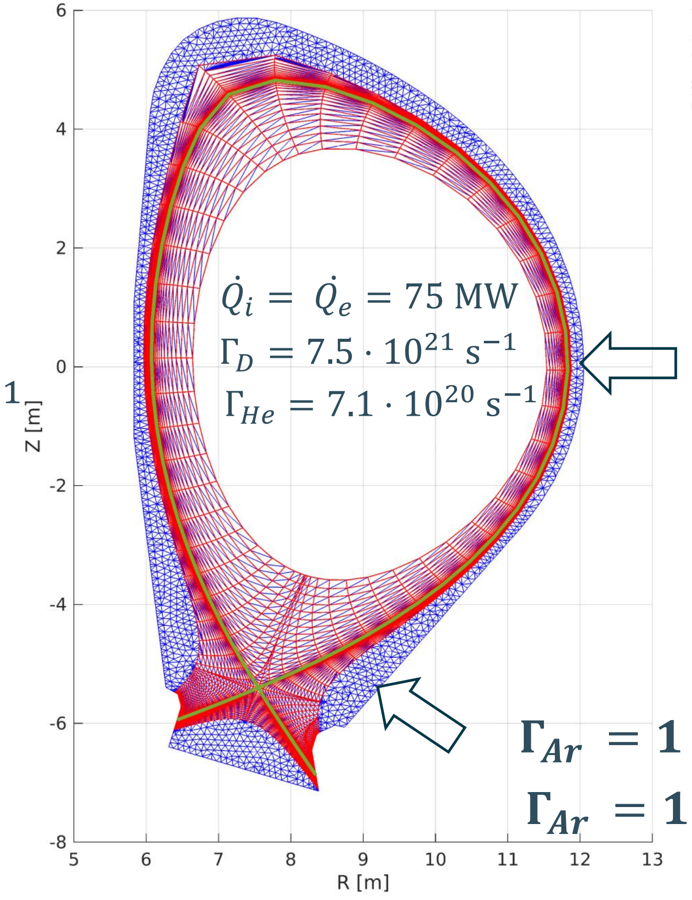
D-only



$T_i = T_e = 1000$ eV
$n_D = 5 \cdot 10^{19}$ m^{-3}

$\Gamma_{D_2} = 1 \cdot 10^{23}$ s^{-1}

D + He + Ar

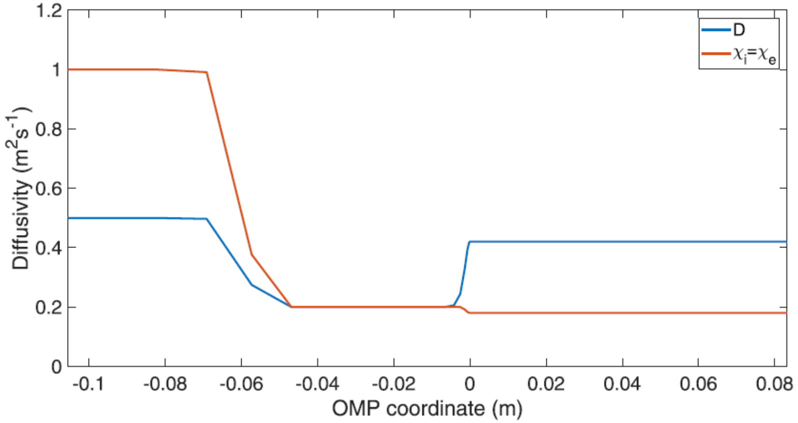


$\dot{Q}_i = \dot{Q}_e = 75$ MW
$\Gamma_D = 7.5 \cdot 10^{21}$ s^{-1}
$\Gamma_{He} = 7.1 \cdot 10^{20}$ s^{-1}

$\Gamma_{D_2} = 1 \cdot 10^{23}$ s^{-1}

$\mathbf{\Gamma_{Ar} = 1 \cdot 10^{19}}$ **s^{-1}**
$\mathbf{\Gamma_{Ar} = 1 \cdot 10^{20}}$ **s^{-1}**

Transport barrier



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D-only: scan on P and Δt

without NNC

P =	760	7.6k	76k	760k
Δt = 1^{e}-4 s				
Δt = 1^{e}-5 s				
Δt = 1^{e}-6 s				
Δt = 1^{e}-7 s				

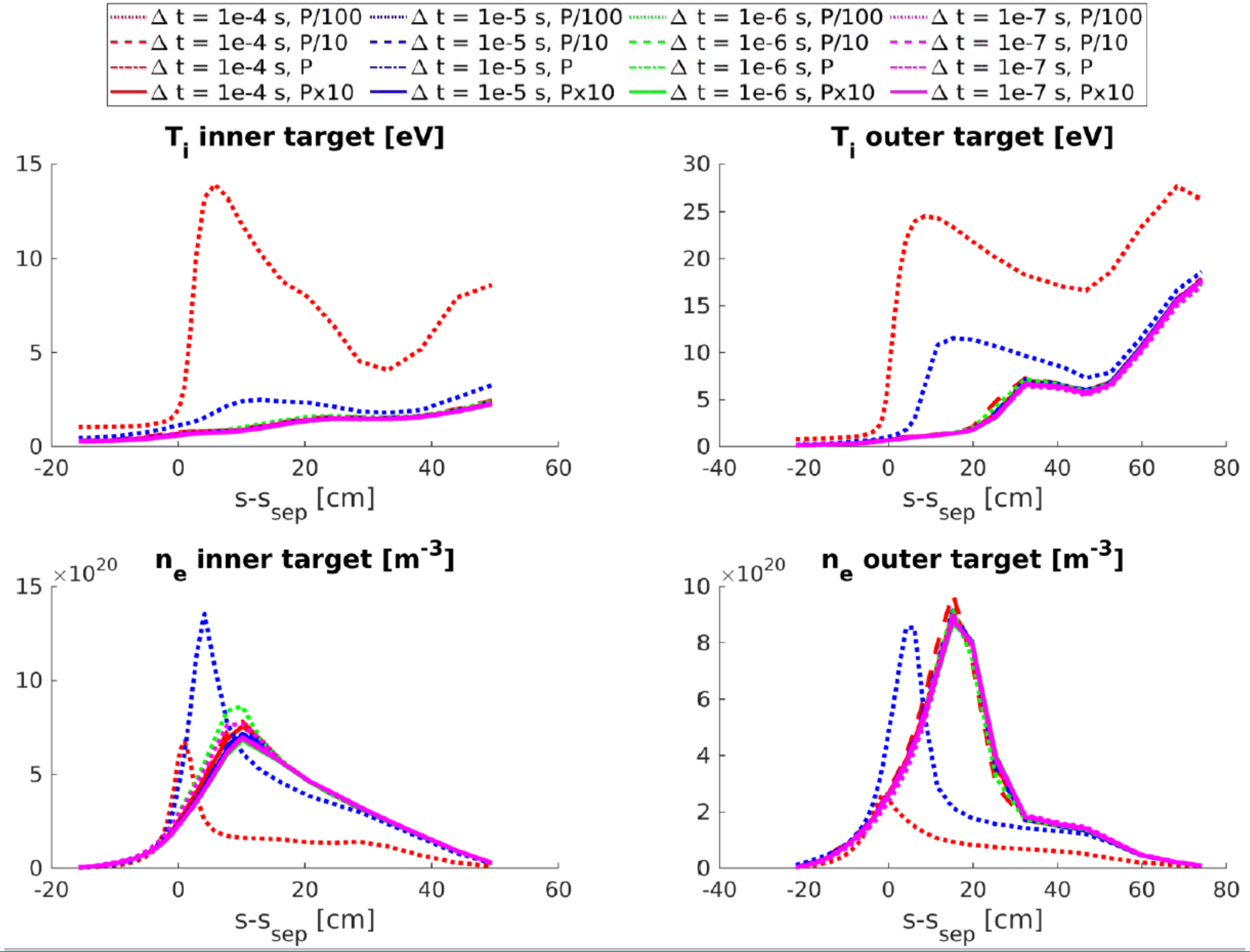
with NNC

P =	760	7.6k	76k	760k
Δt = 1^{e}-4 s				
Δt = 1^{e}-5 s				
Δt = 1^{e}-6 s				
Δt = 1^{e}-7 s				

Location	$P_{original}$
Inner target	25000
Outer target	25000
Inner PFR	2000
Outer PFR	2000
MCW	2000
Vol. Rec.	10000
Gas puff	10000

Q1: effect of Δt on bias?
Q2: effect of NNC on error scaling?

D-only results (with NNCs)



Only 1^e-4s and 1^e-5s for P/100 lead to a qualitatively wrong solution

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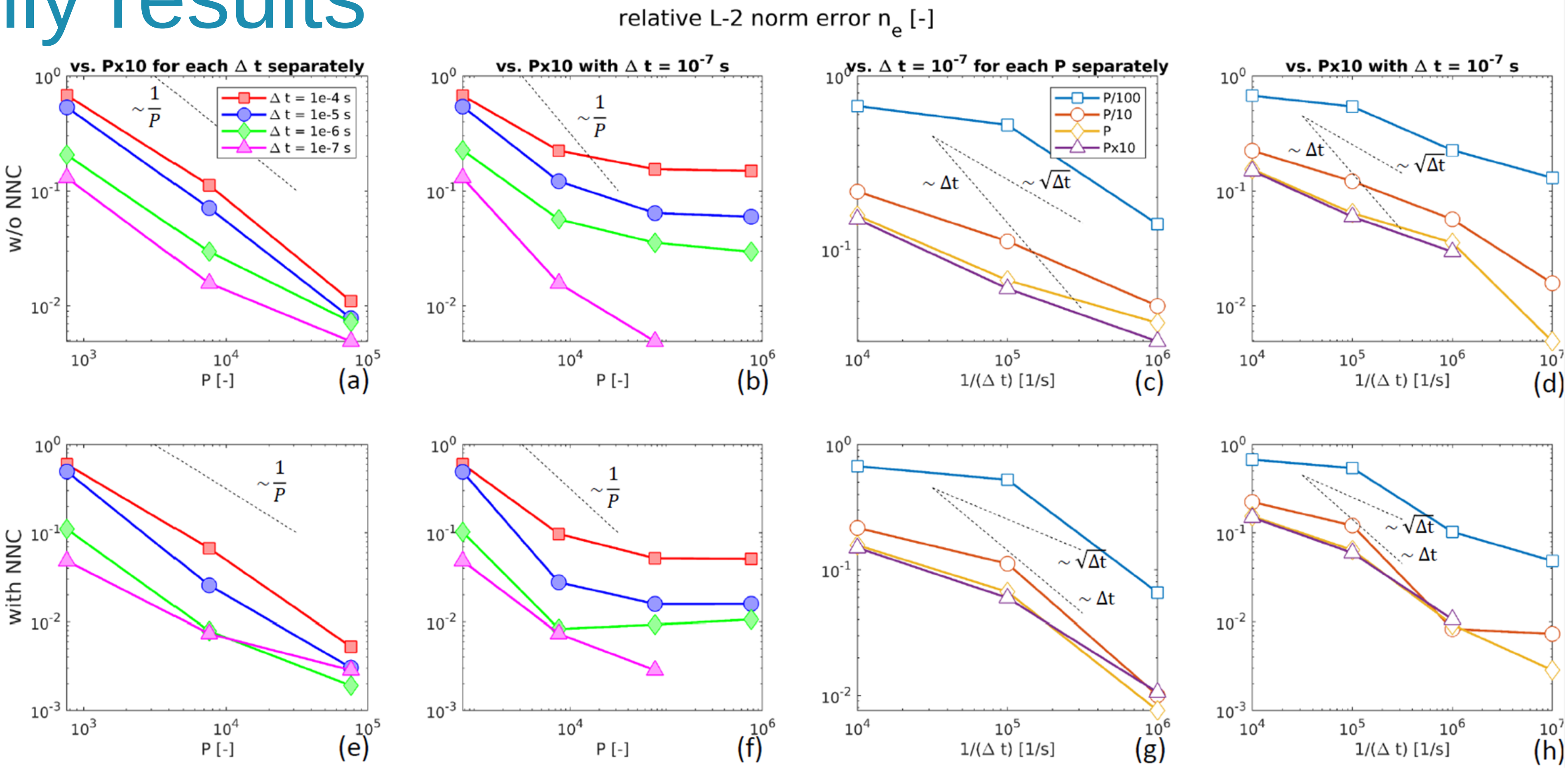
D-only results



→ no noticeable effect of NNCs on convergence behavior
→ bias decreases monotinically with Δt

Choice for number of impurity MC particles

Impurity neutrals ≈ 1 order of magnitude smaller CPU time/particle than D/D_2
→ Chose similar CPU time per stratum for impurities

Location	D
Inner target	25000
Outer target	25000
Inner PFR	2000
Outer PFR	2000
MCW	2000
Vol. Rec.	10000
Gas puff	10000

Location	D	He	Ar
Inner target	25000	250000	250000
Outer target	25000	250000	250000
Inner PFR	2000	20000	20000
Outer PFR	2000	20000	20000
MCW	2000	20000	20000
Vol. Rec.	10000	100000	100000
Gas puff	10000	/	100000

Scans on D+He+Ar cases

With NNCs

Ar puff 1^{e}19 /s

P =	130k	1.3M	13M
Δt = 1^{e}-4 s			
Δt = 1^{e}-5 s			
Δt = 1^{e}-6 s			
Δt = 1^{e}-7 s			

Ar puff 1^{e}20/s

P =	130k	1.3M	13M
Δt = 1^{e}-4 s			
Δt = 1^{e}-5 s			
Δt = 1^{e}-6 s			
Δt = 1^{e}-7 s			

Without NNCs

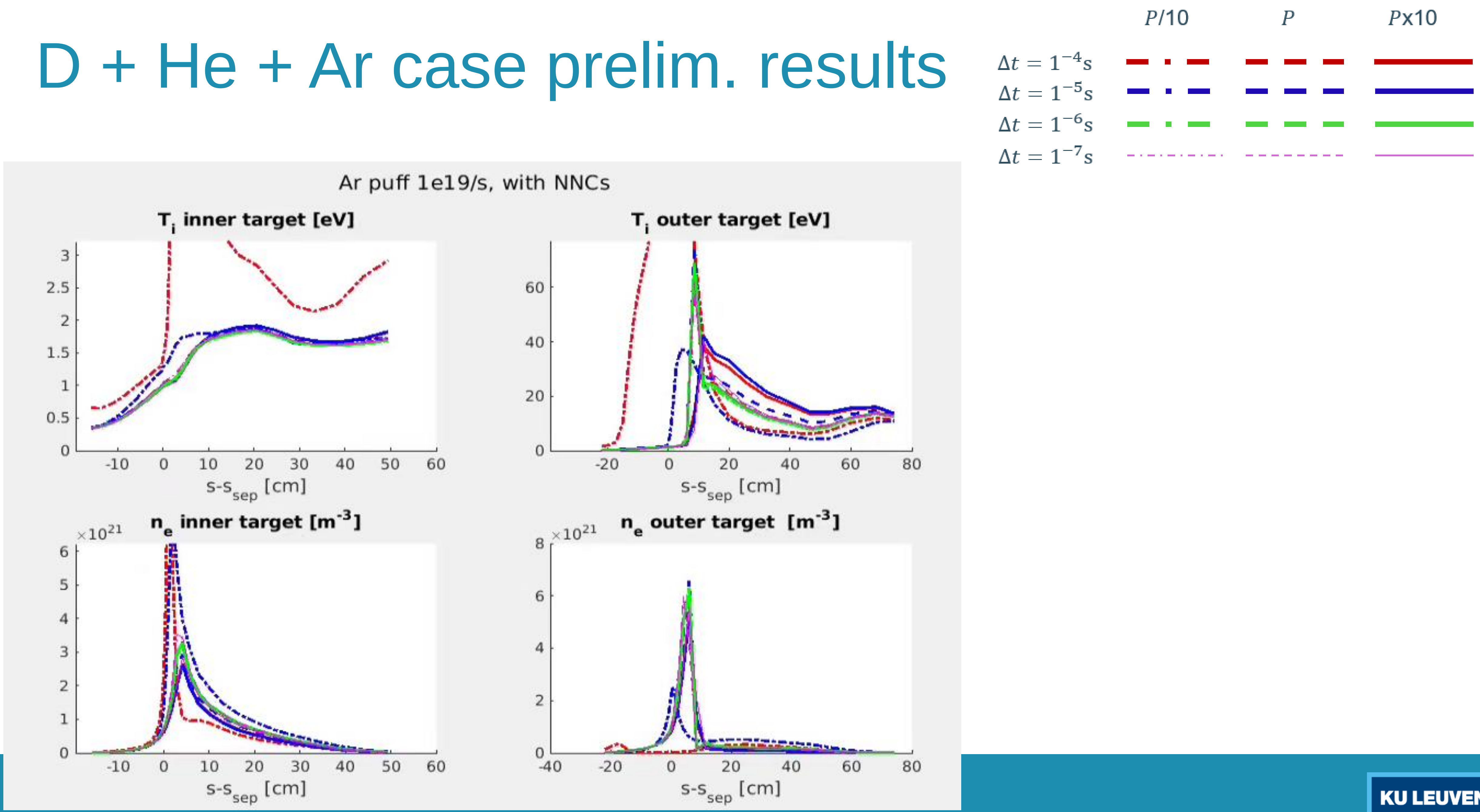
Ar puff 1^{e}19 /s

P =	130k	1.3M	13M
Δt = 1^{e}-4 s			
Δt = 1^{e}-5 s			
Δt = 1^{e}-6 s			
Δt = 1^{e}-7 s			

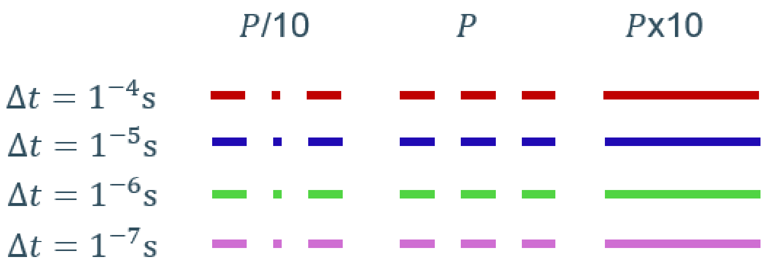
Ar puff 1^{e}20/s

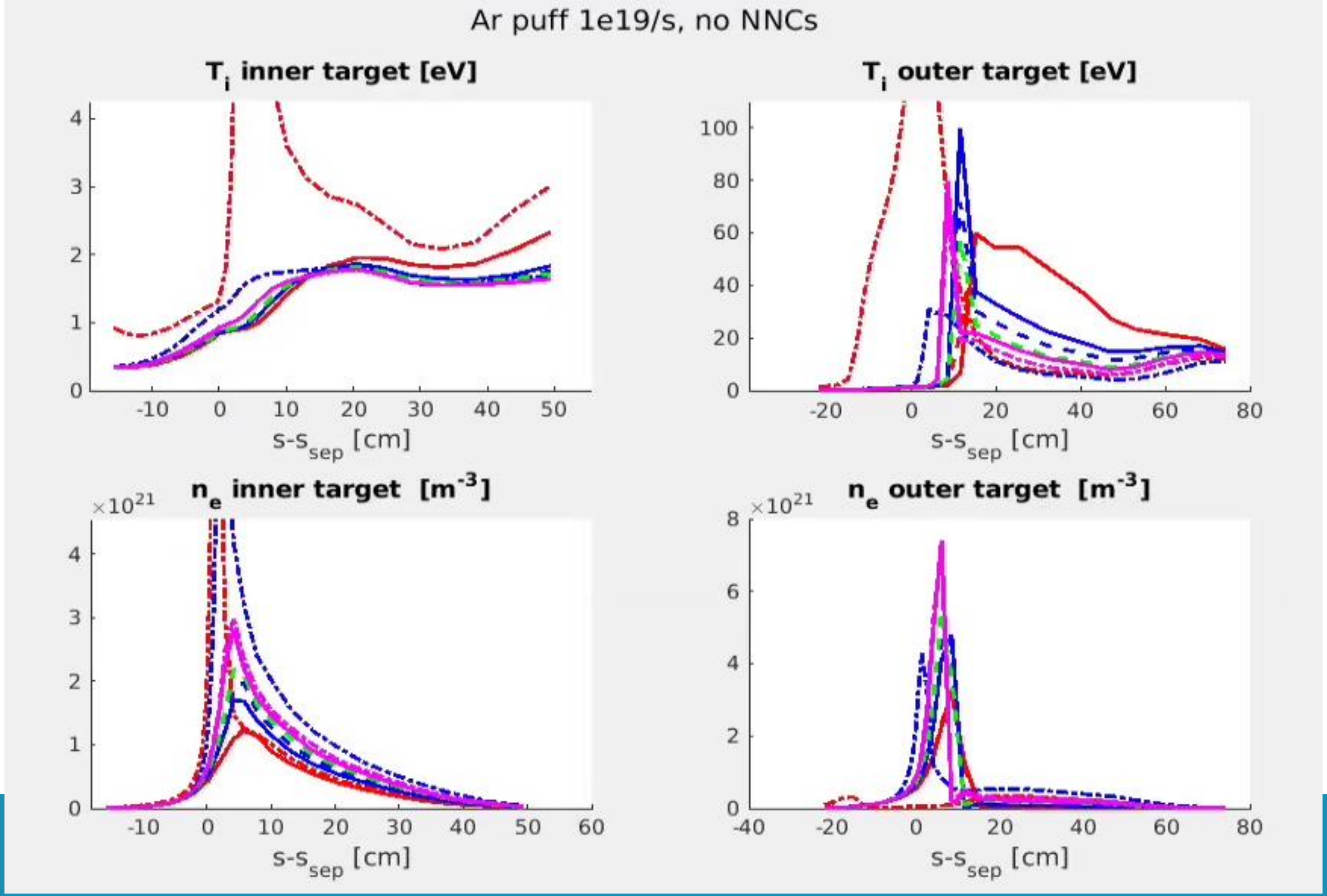
P =	130k	1.3M	13M
Δt = 1^{e}-4 s			
Δt = 1^{e}-5 s			
Δt = 1^{e}-6 s			
Δt = 1^{e}-7 s			

D + He + Ar case prelim. results

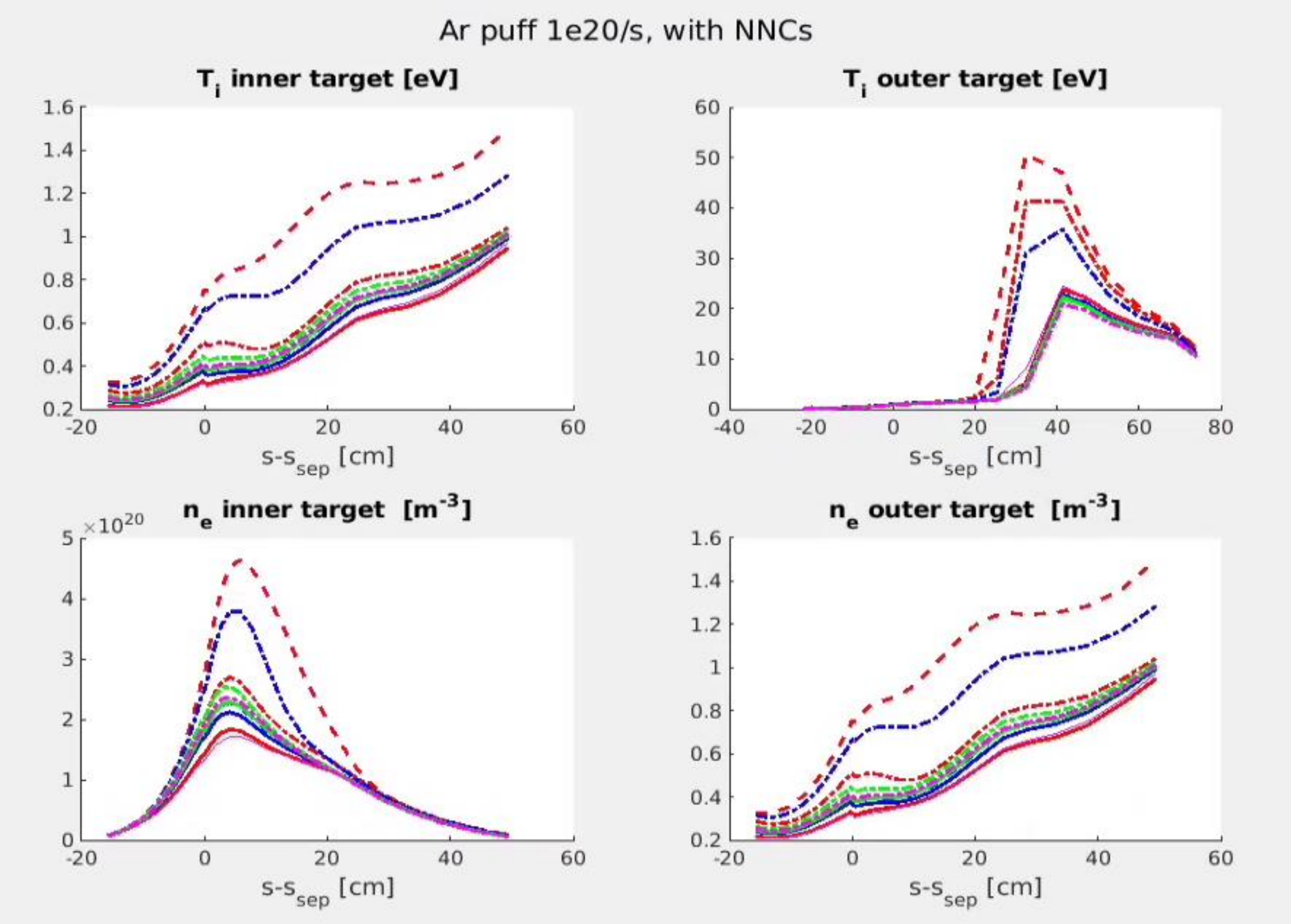


D + He + Ar case prelim. results



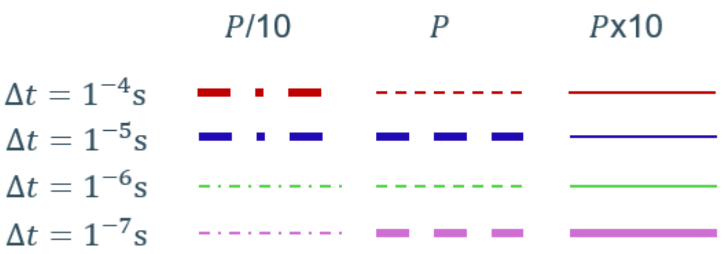


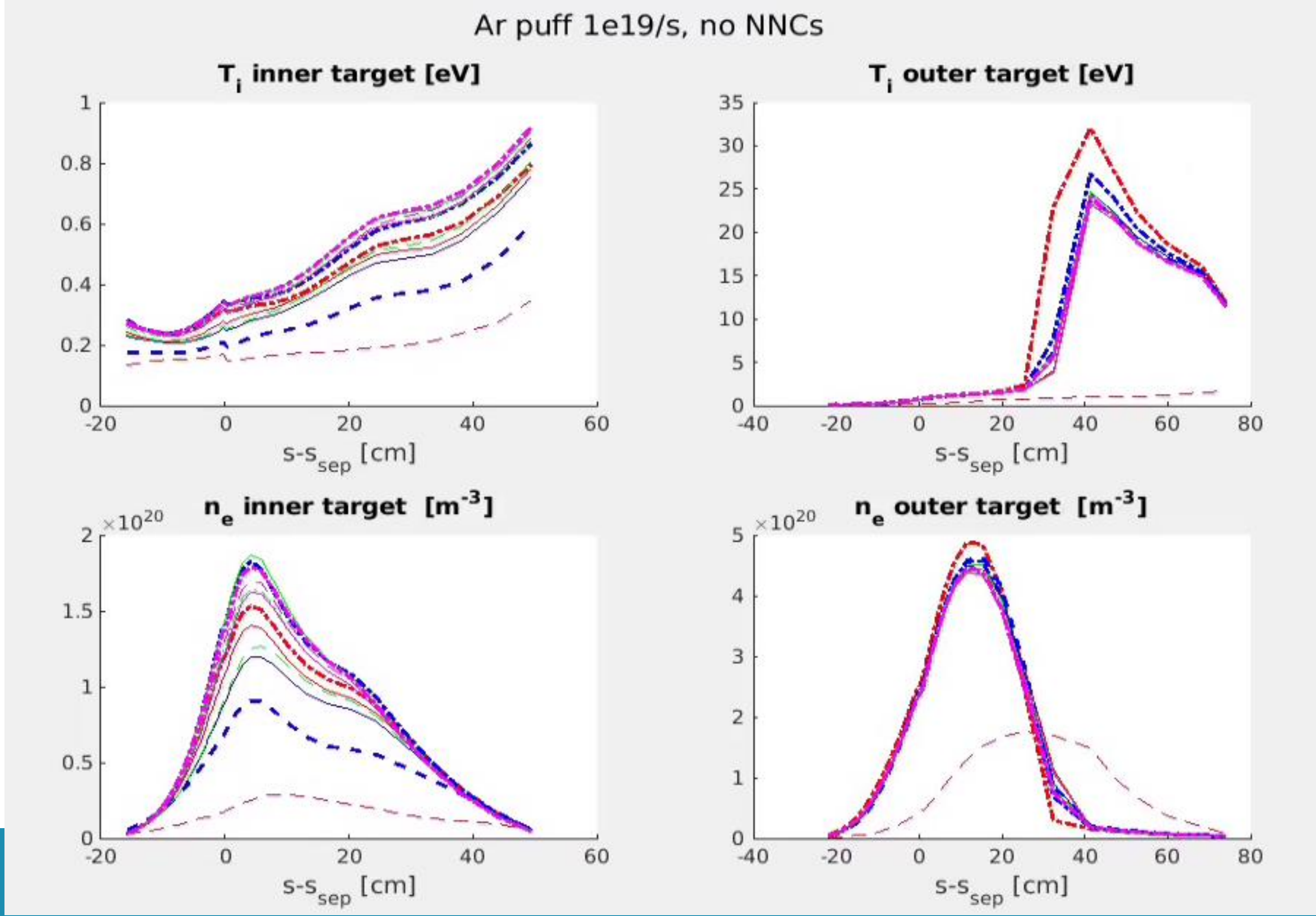
D + He + Ar case prelim. results



	$P/10$	P	Px10
$\Delta t = 1^{-4}$s			
$\Delta t = 1^{-5}$s			
$\Delta t = 1^{-6}$s			
$\Delta t = 1^{-7}$s			

D + He + Ar case prelim. results

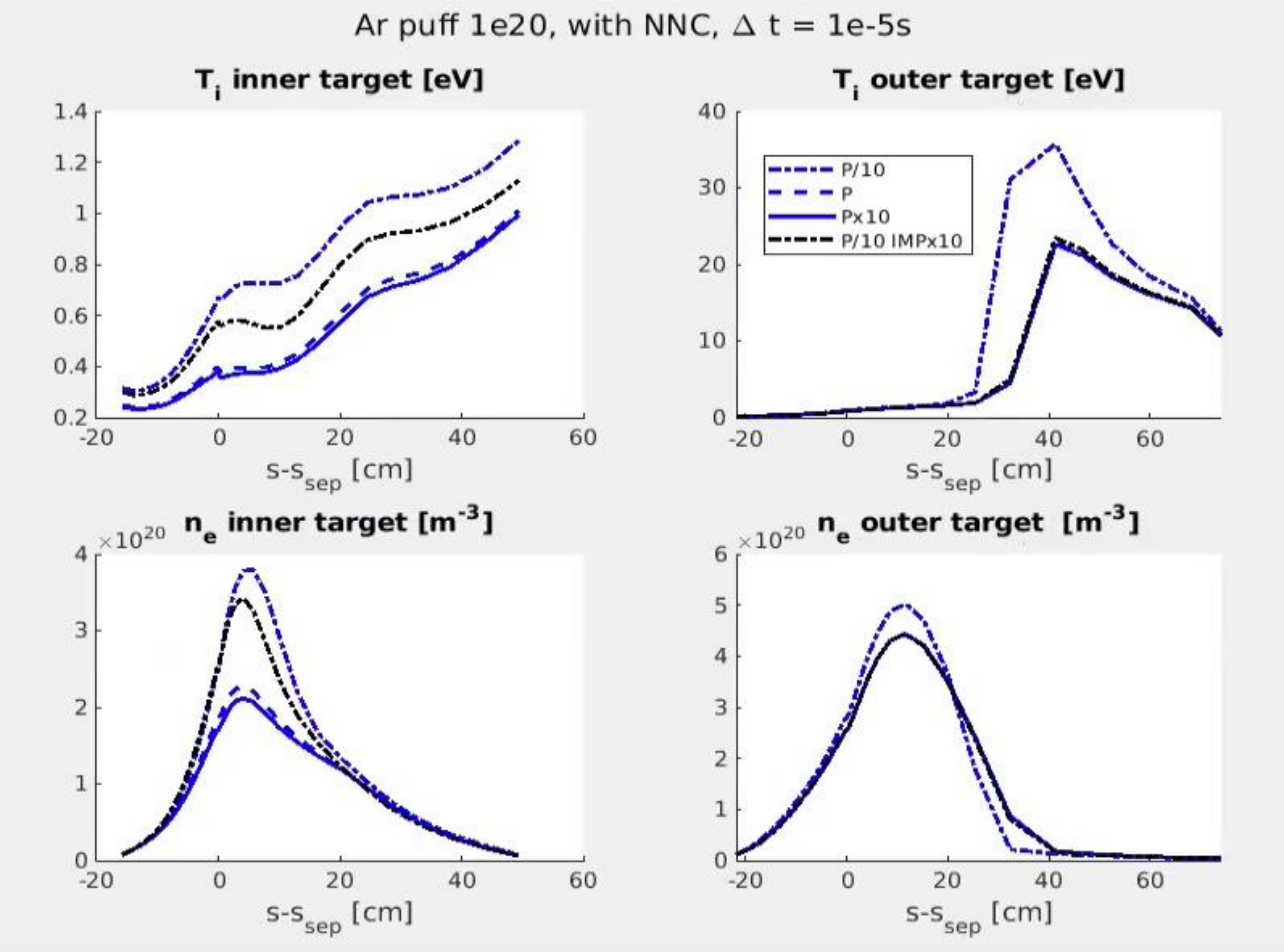




Prelim. conclusions D + He + Ar cases

- Multi-species cases appear to have much larger bias than D-only case
- Why?
  - Purely case dependent? E.g. much higher core power? higher T’s OT?
  - Bad statistics from impurity neutrals themselves?
  - Combination of both?

Experiment: multiply only impurities again x10



IT:
bias decreases but not /10

OT:
solution collapses onto P and Px10
→ bias originated from impurities themselves

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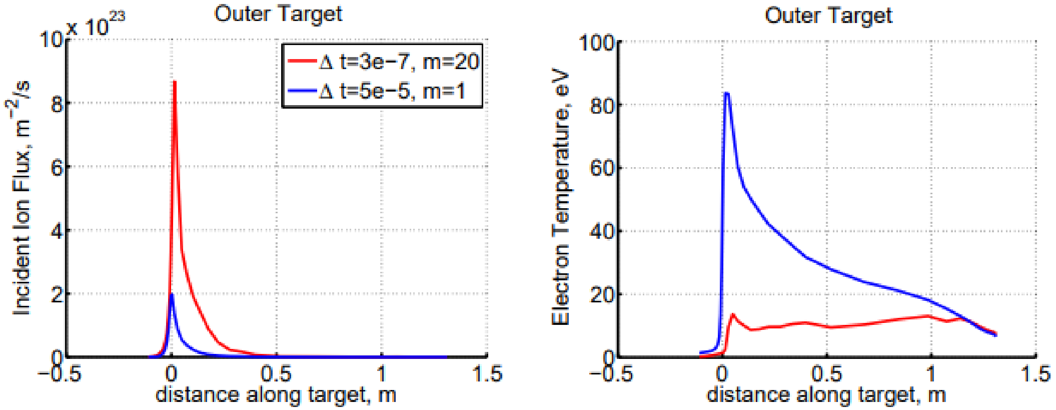
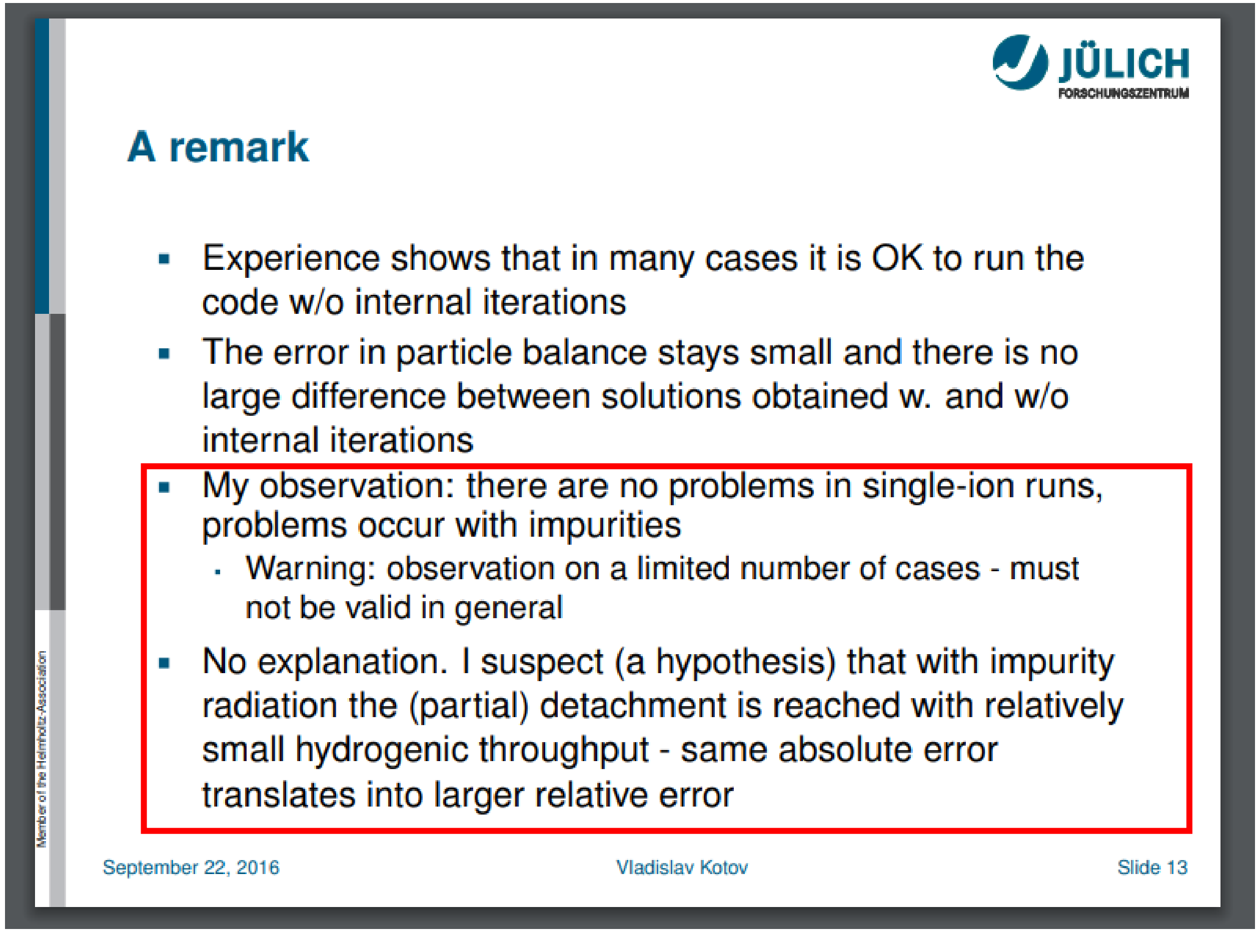
Similar observations in literature

Non-local effect of saturated residuals in B2-EIRENE (SOLPS) simulations September 22, 2016 Vladislav Kotov

presentation linked to

Kotov, Vladislav. "Particle conservation in numerical models of the tokamak plasma edge." *Physics of Plasmas* 24.4 (2017).





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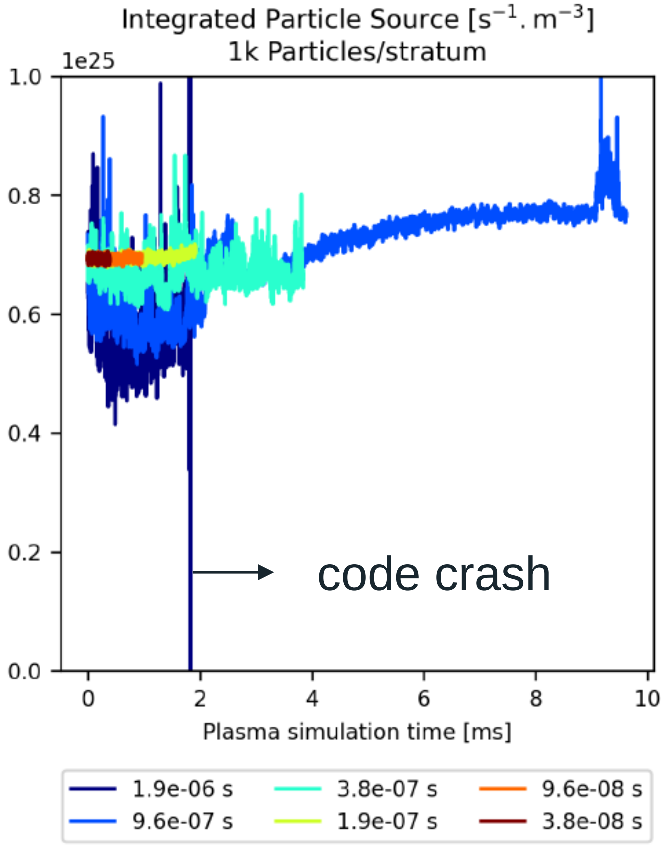
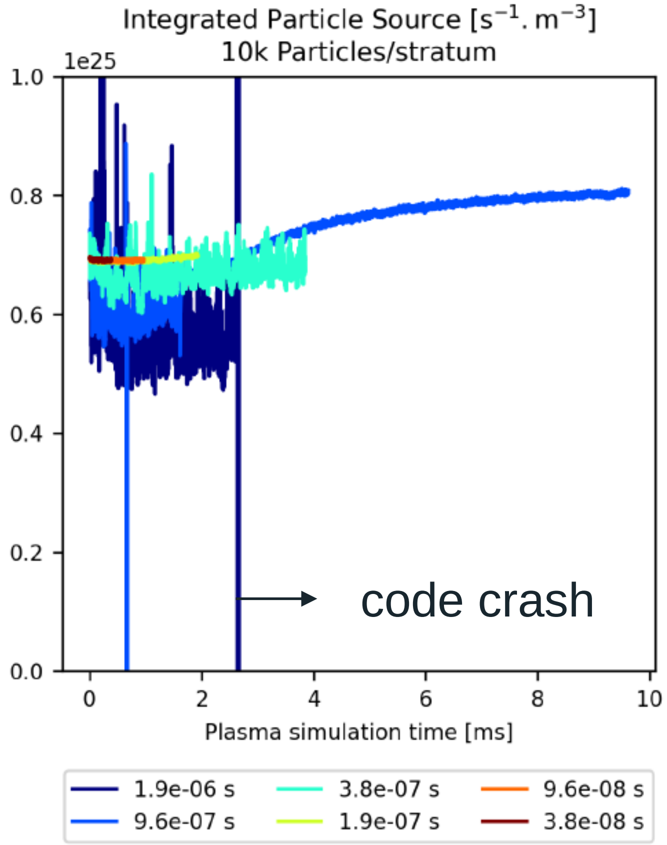
Similar observations in literature

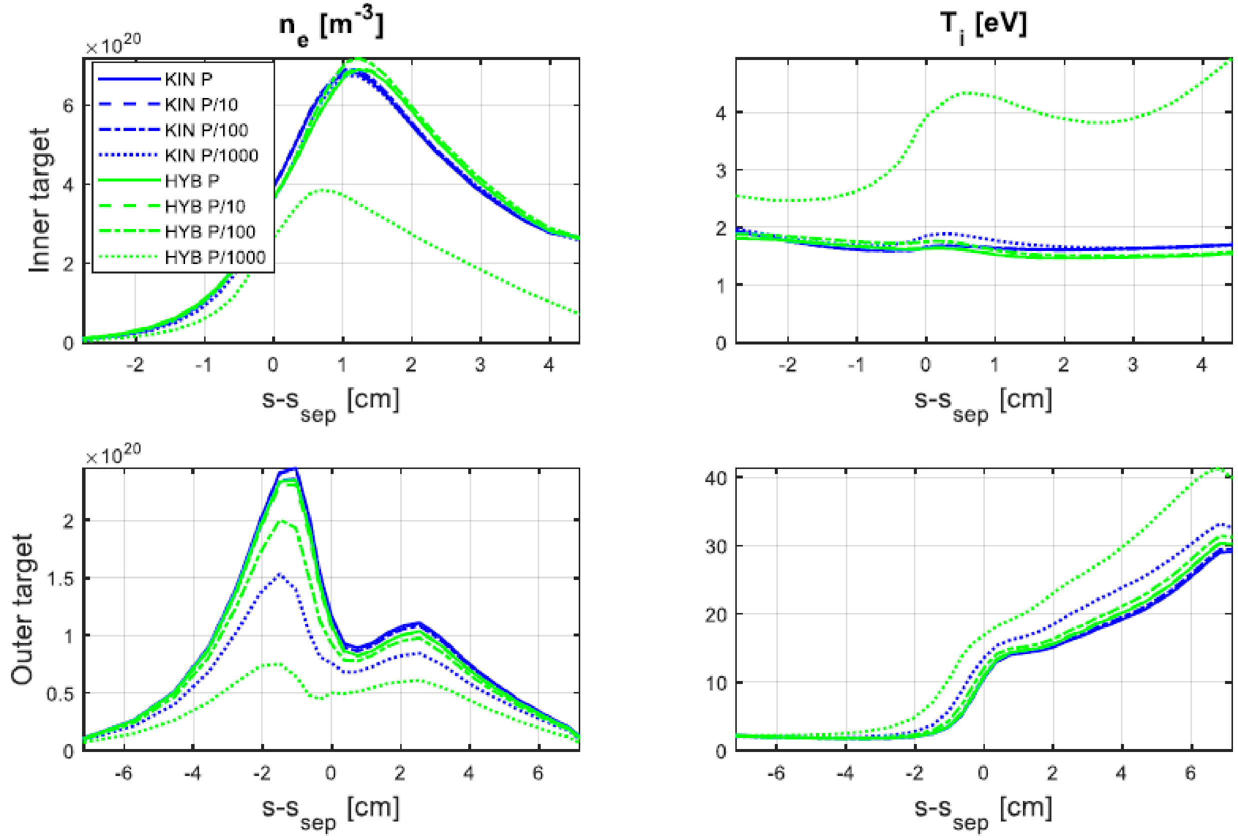
- PhD N. Rivals + communications at PSI
  - In SOLEDGE3X, very strict time-step limitations found for ITER D + Ne + He cases
  - Much less issues for D-only





Similar observations in literature

- Own spatially hybrid results (= multi-species case with fluid ions and fluid neutrals)



Proportional particle distribution			
Source	Type	KIN	$\mathrm{HYB}-2:\mathrm{Kn}^t=10$
IT	$\Gamma^{fl\to k}_{i,inc}$	38000	38000
	$\Gamma^{fl\to k}_{a,inc}$	/	140000
OT	$\Gamma^{fl\to k}_{i,inc}$	32000	32000
	$\Gamma^{fl\to k}_{a,inc}$	/	1200
I. PFR	$\Gamma^{fl\to k}_{i,inc}$	1000	1000
	$\Gamma^{fl\to k}_{a,inc}$	/	6100
O. PFR	$\Gamma^{fl\to k}_{i,inc}$	1000	1000
	$\Gamma^{fl\to k}_{a,inc}$	/	1000
MCW	$\Gamma^{fl\to k}_{i,inc}$	44000	44000
	$\Gamma^{fl\to k}_{a,inc}$	/	80000
Vol. rec.	$\Gamma_{i\to a}$	10000	/
Total		126000	344300
Ratio			2.73

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Conclusions

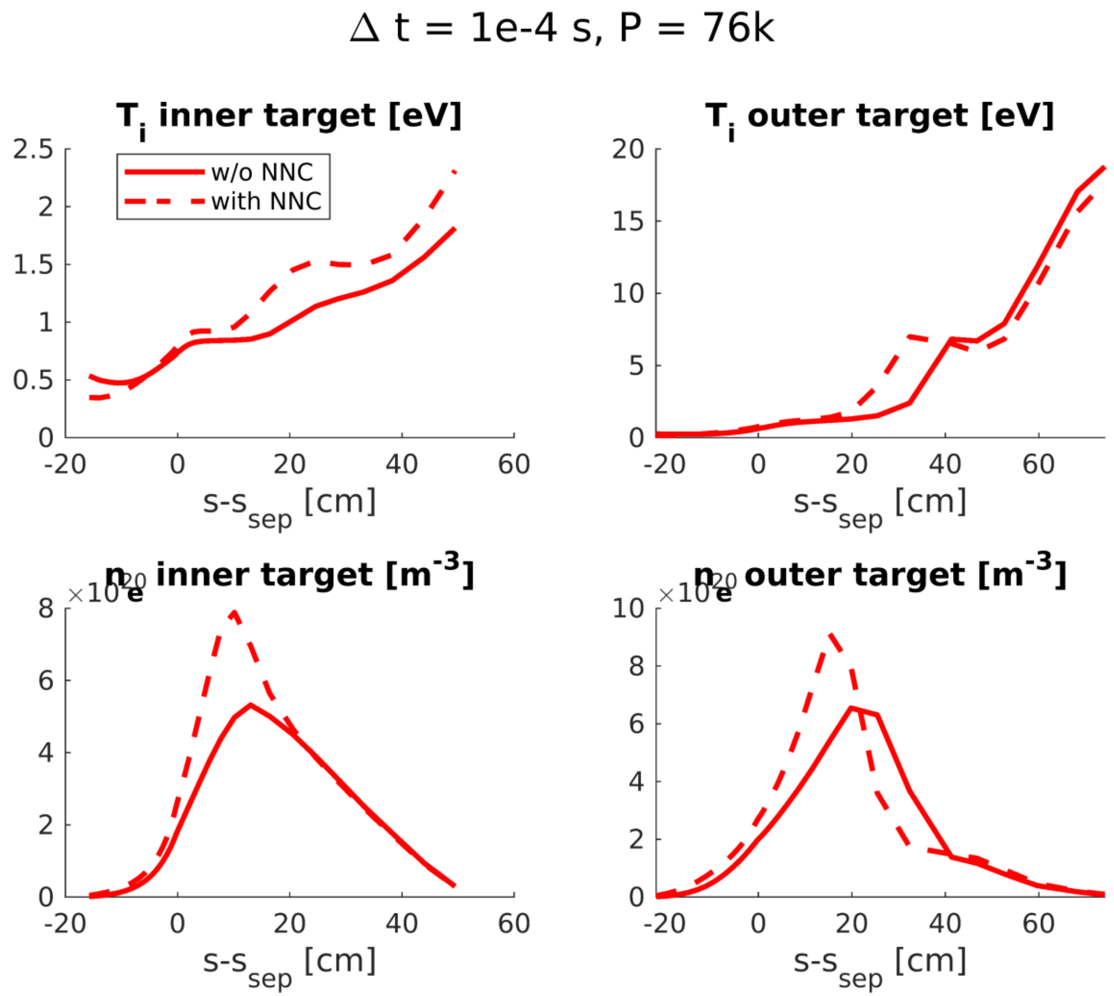
- Error reduction w.r.t. P and Δt does not change significantly with NNCs
- Decrease of bias for smaller Δt demonstrated in SOLPS-ITER
  - useful knowledge if Δt is limited by plasma side (e.g. drifts)
- Bias error seems to be much higher for (high-power?) multi-species cases
  - Similar observations in literature
  - Need to better understand why
  - Optimal strategies for D-only may no longer be optimal

$\rightarrow$ high priority for future research
$\rightarrow$ back to 1D or slab cases? DEMO cases much too slow for efficient research

Back-up

D-only results: effect of NNC

- Noticeable effect
- Same regime



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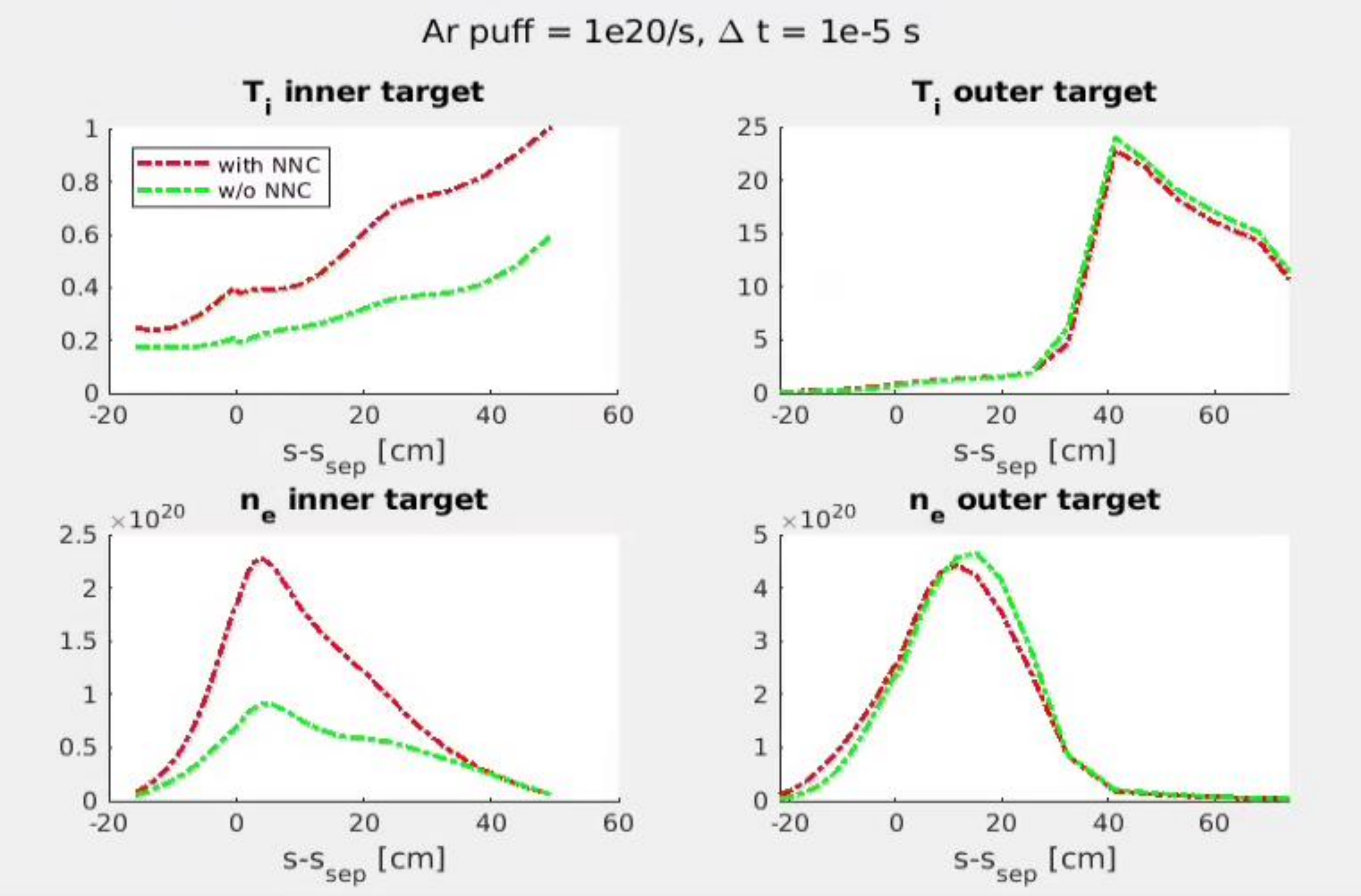
D+He+Ar: effect of NNC



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Q3: how to set P_{imp} vs P_D?

	D/D_2	He	Ar
Source [s^{-1}]	$1{,}56 \cdot 10^{25}$	$1{,}16 \cdot 10^{23}$	$1{,}19 \cdot 10^{22}$
CPUt / P [μs]	$735{,}6$	$71{,}9$	$35{,}4$

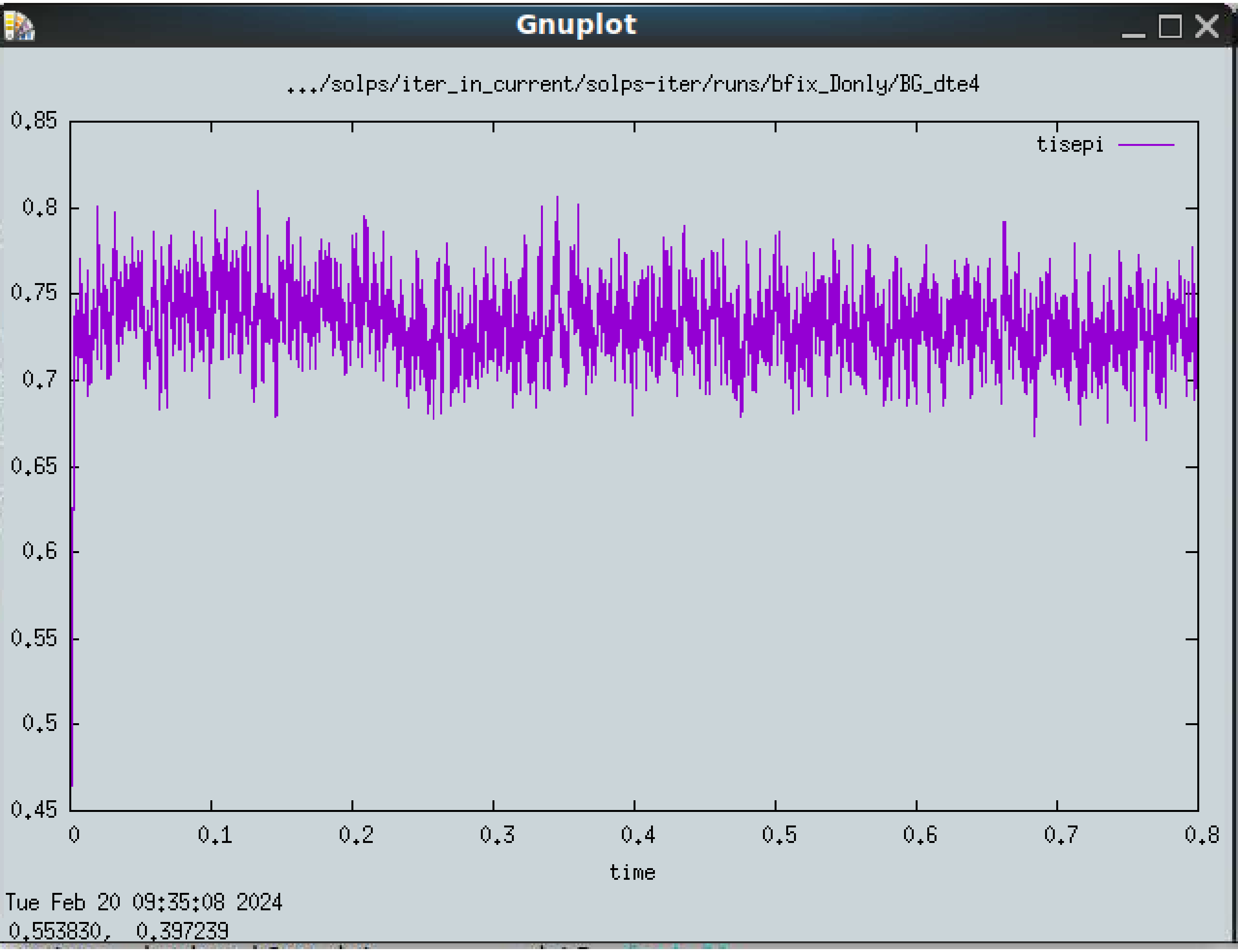
- physical flux is 2-3 orders of magnitude smaller for impurities, but large effect on energy balance
- impurities are $\pm$ 1 order of magnitude faster per MC particle

→ nothing to gain by setting $P_{imp} < P_D$
→ either $P_{imp} \approx P_D$ or $P_{imp} > P_D$

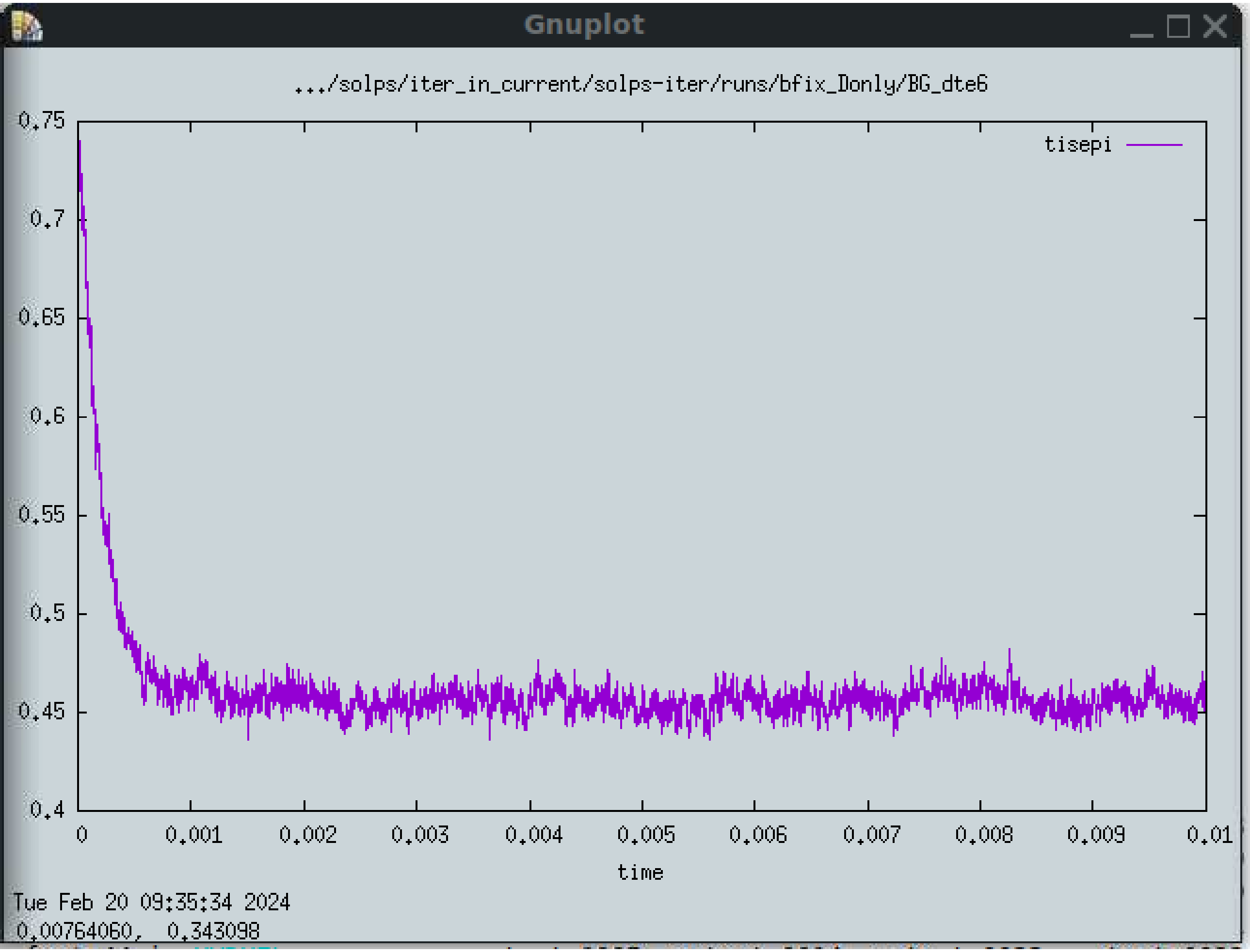
Q3: how to set P_{imp} vs P_D?

- Choose a Δt and P_D that gave low error for D-only
- Check with $P_{imp} = \frac{P_D}{10}, P_{imp} = P_D$, and $P_{imp} = P_D \cdot 10$
- No results yet

Run with $\Delta t = 10^{-4}s$ starting from $\Delta t = 10^{-6}s$ solution

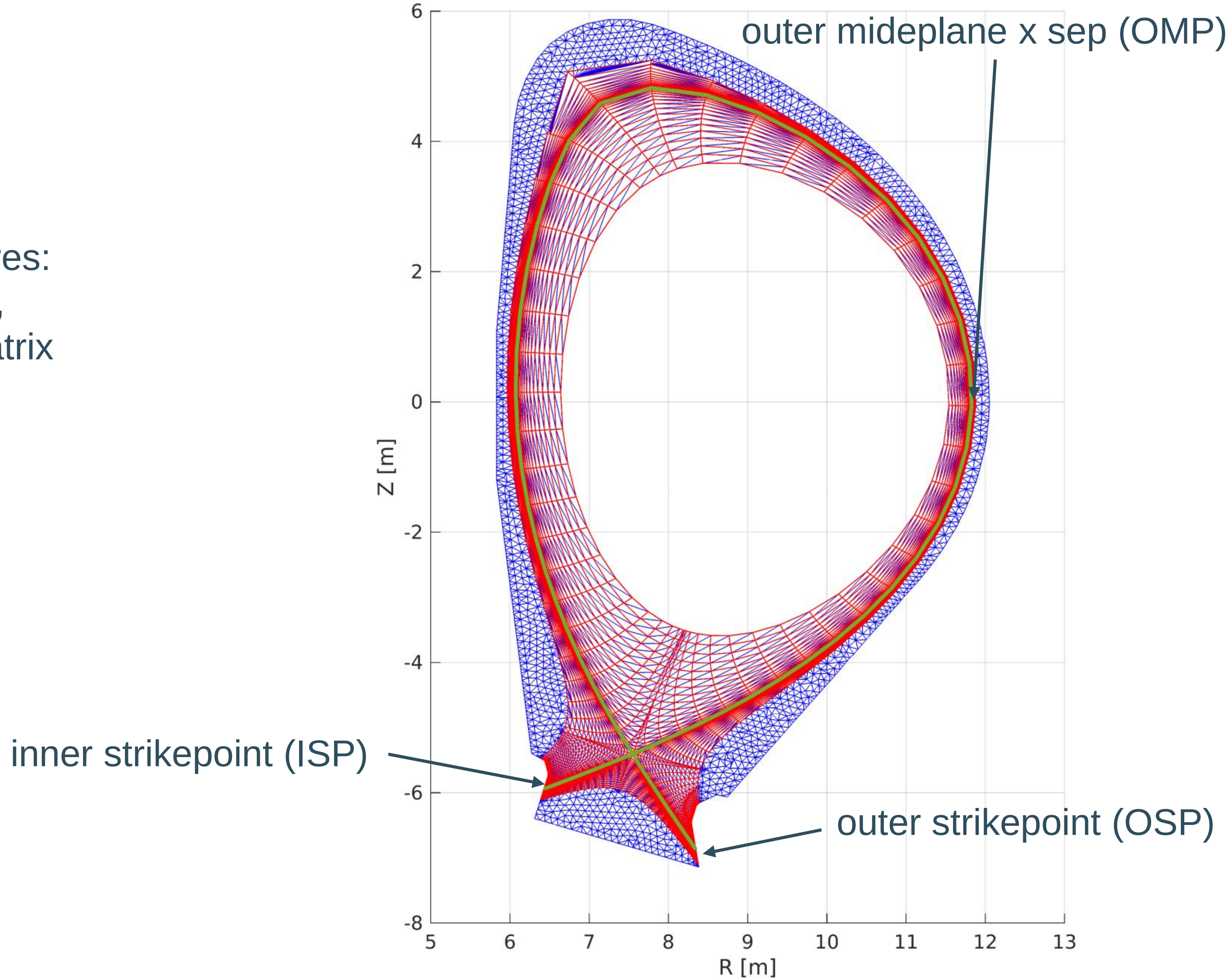


Run with $\Delta t = 10^{-6}s$ starting from $\Delta t = 10^{-4}s$ solution



Results D-only

Will show scalar results to reduce figures: ion density and ion temperature at ISP, OSP, and crossing of OMP and separatrix



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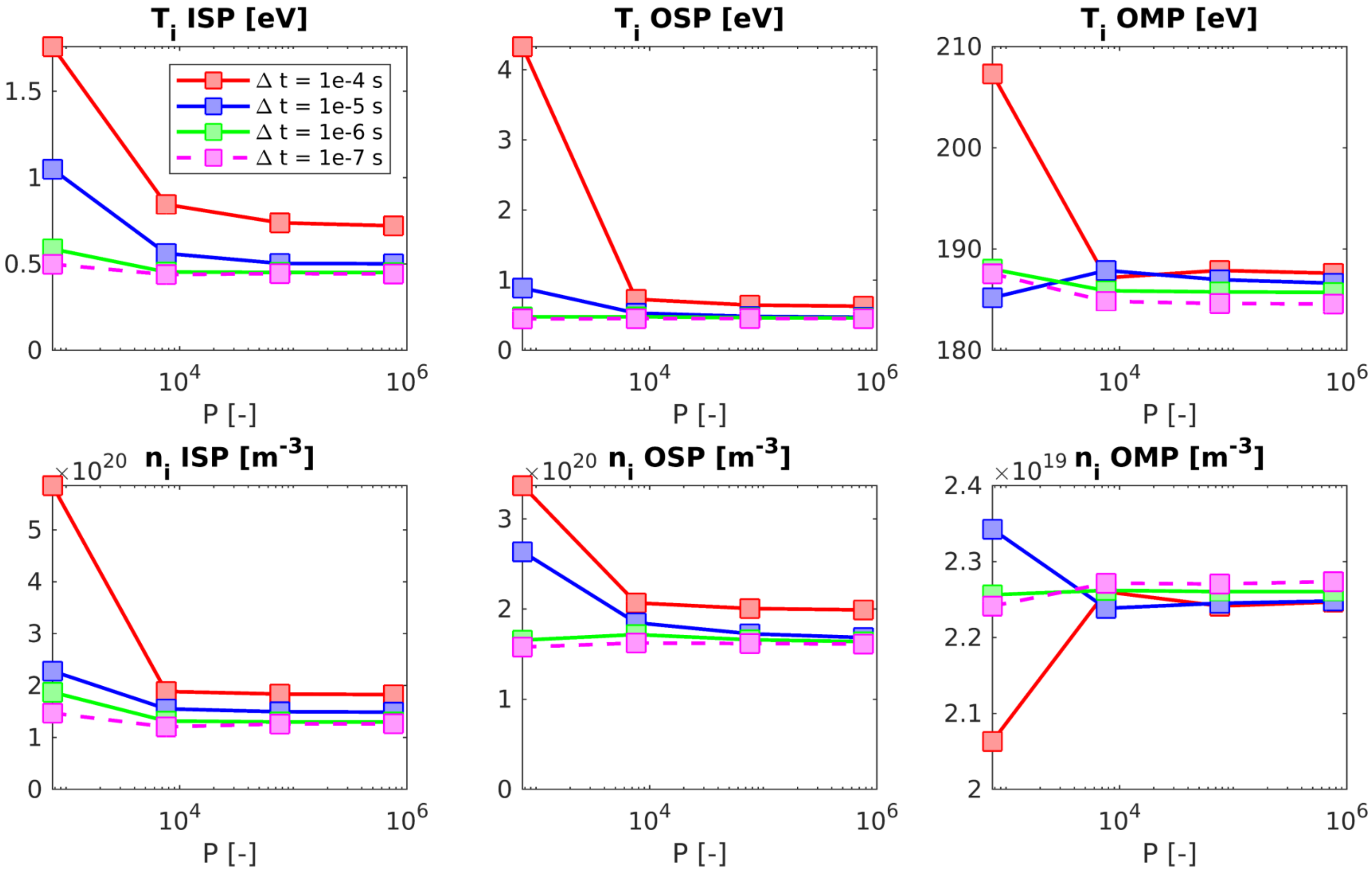
Results D-only

- Error decreases with P ↑
- Error decreases with Δt ↓
- Different Δt's converge to different solution for P → ∞ ??

w.o. NNC



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Results D-only

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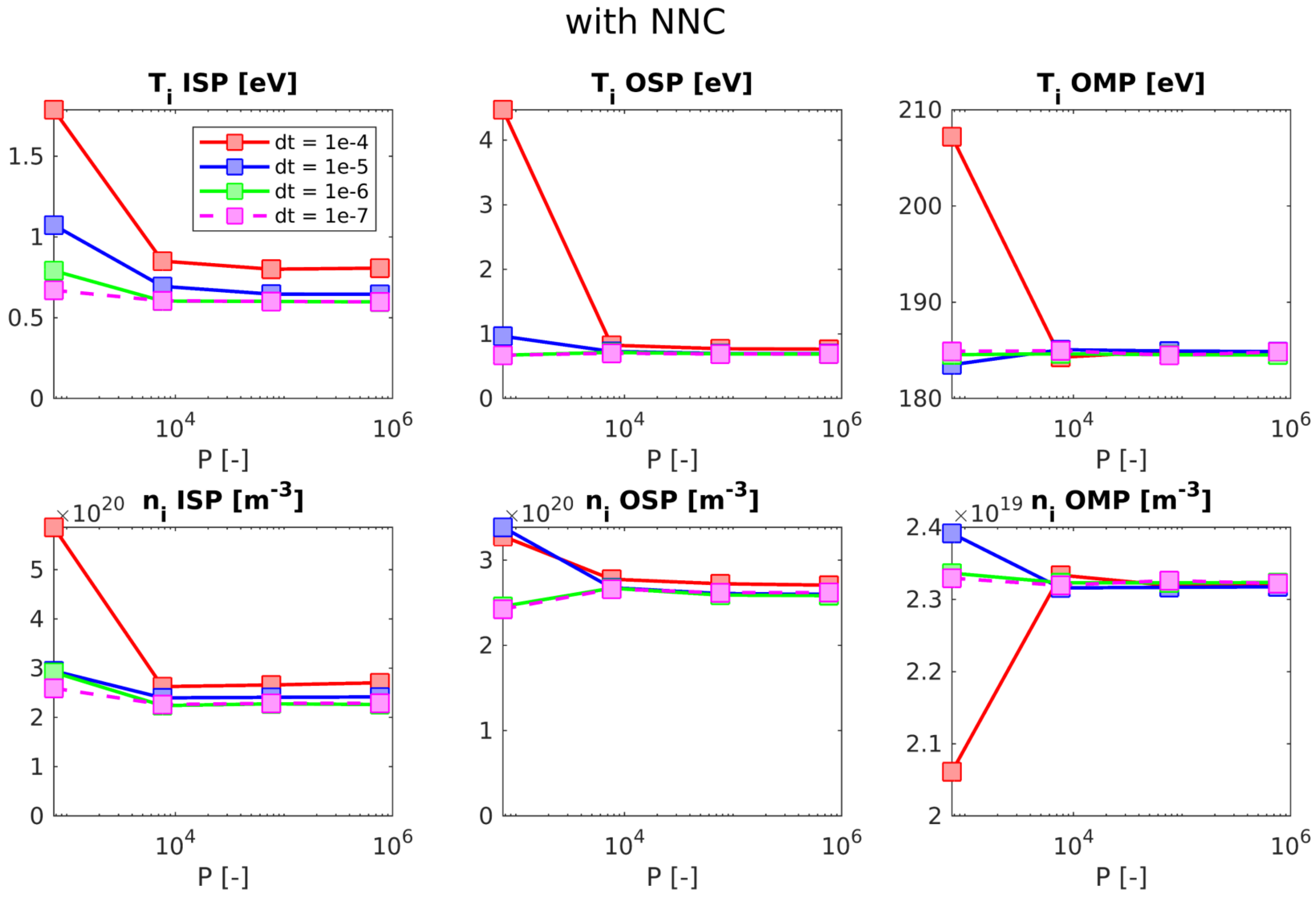

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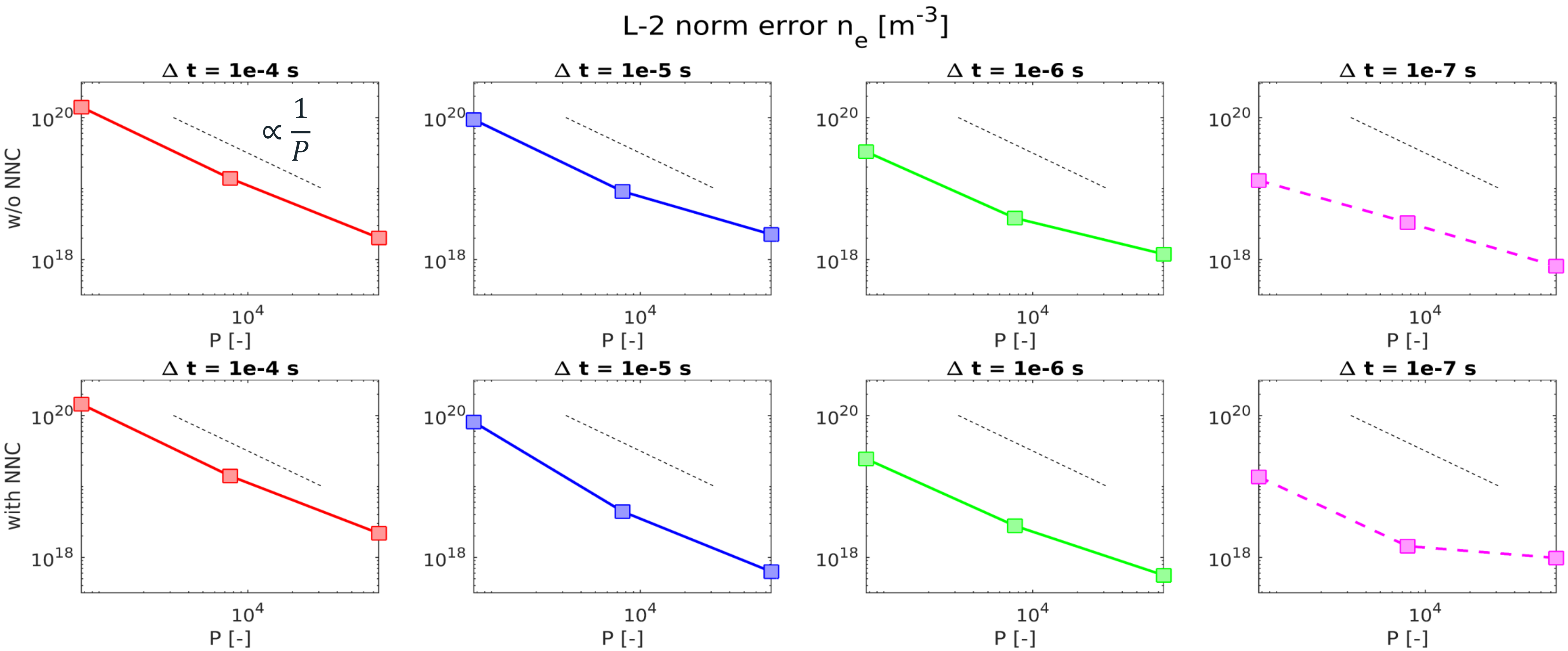
D-only results

- Error scaling if we assume that Px10 is exact solution, for each Δt separately



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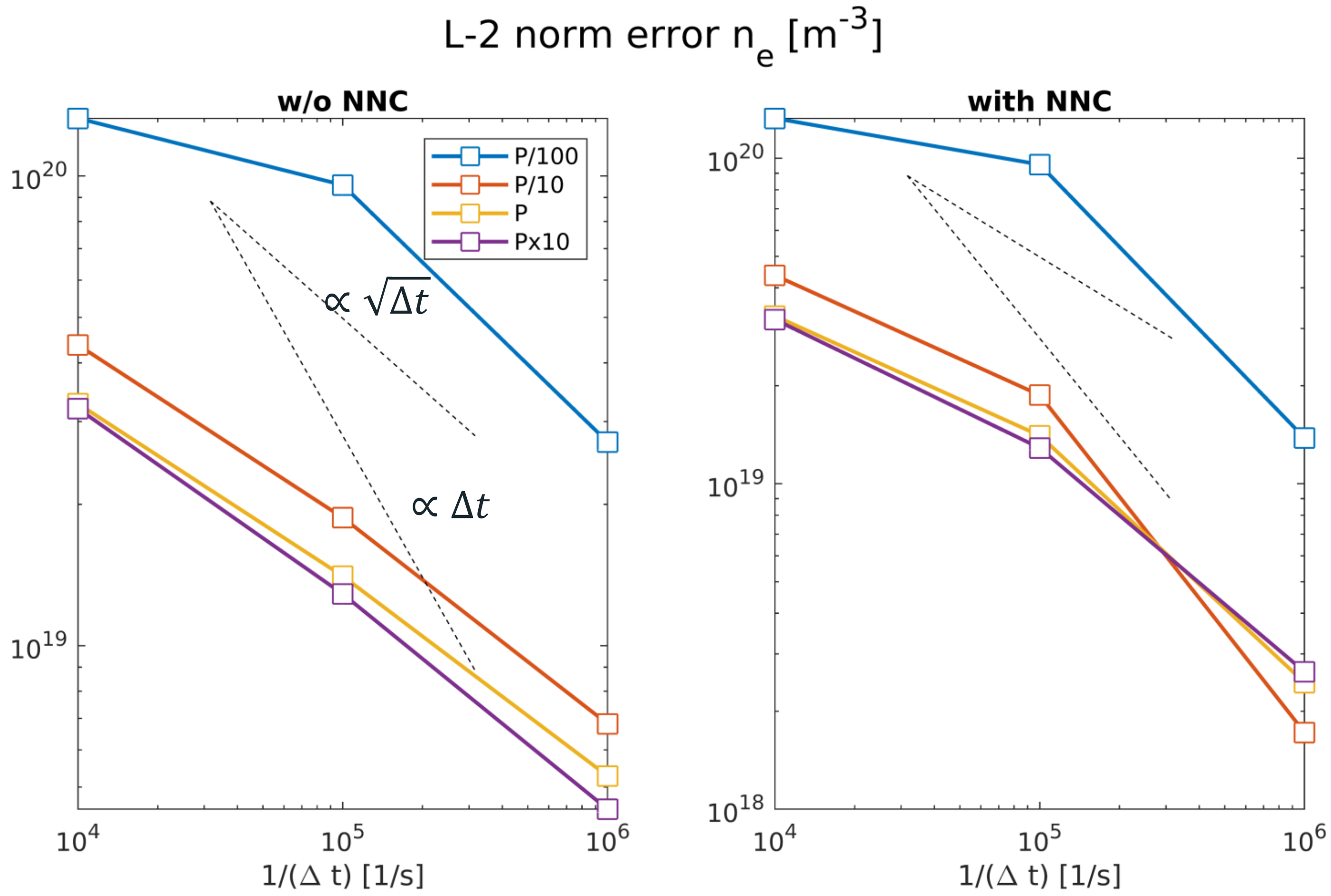
Impurity seeding

- ITER and DEMO will rely heavily on seeded impurities
- e.g. Neon, Argon
- Cause radiative cooling of plasma
- Balance between cooling of edge and contamination of core

D-only results

- Error scaling if we assume that $\Delta t = 10^{-7}$ is exact solution, for each P separately



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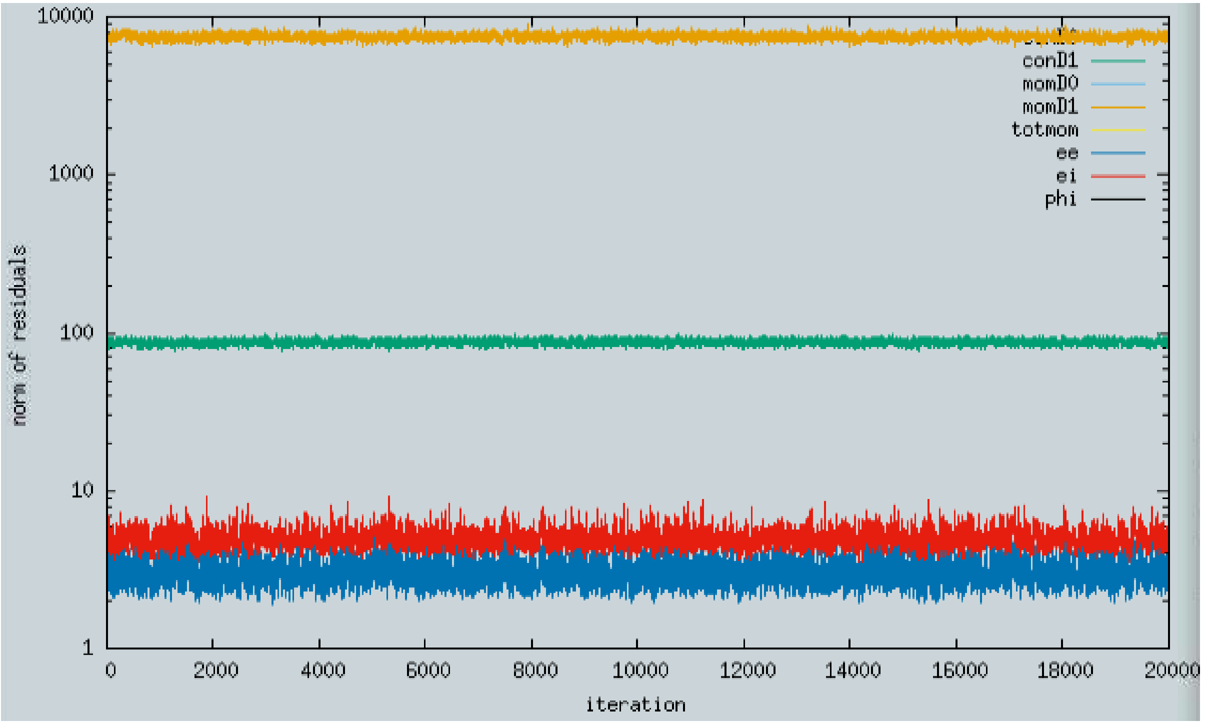
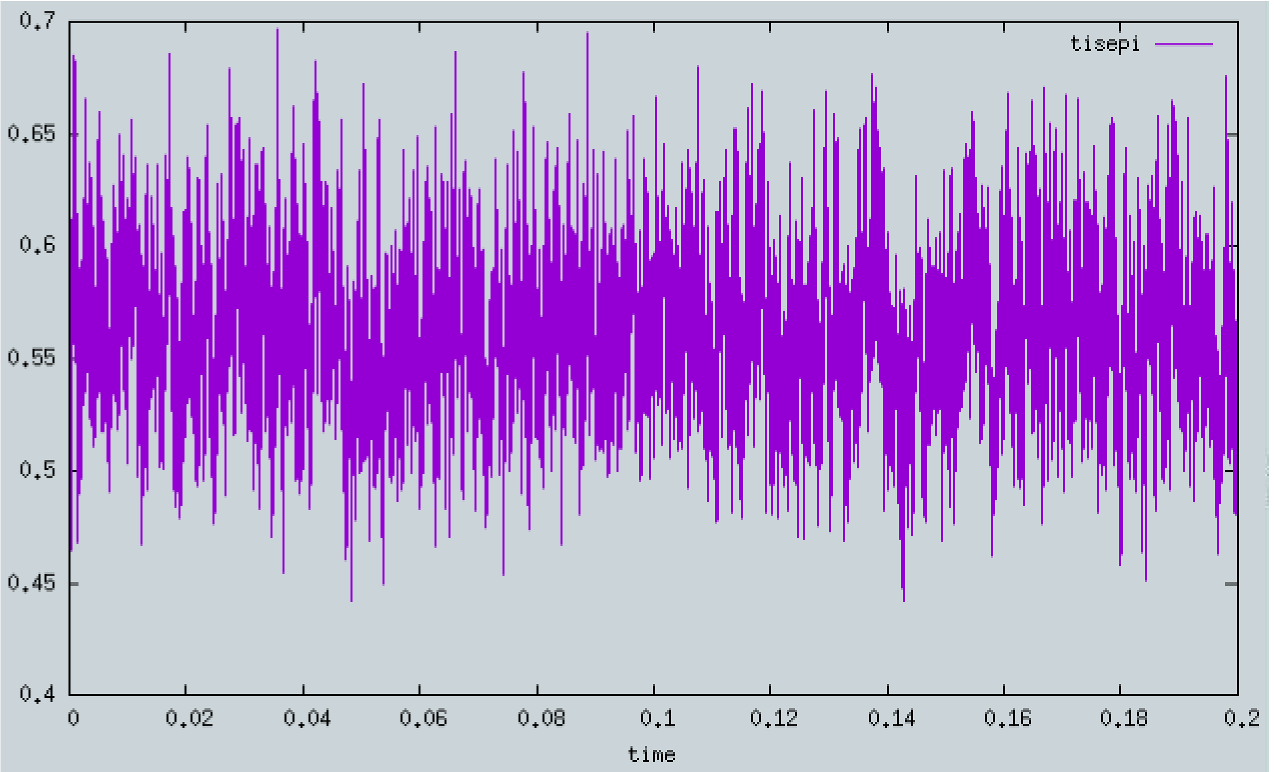
B2.5-EIRENE coupling

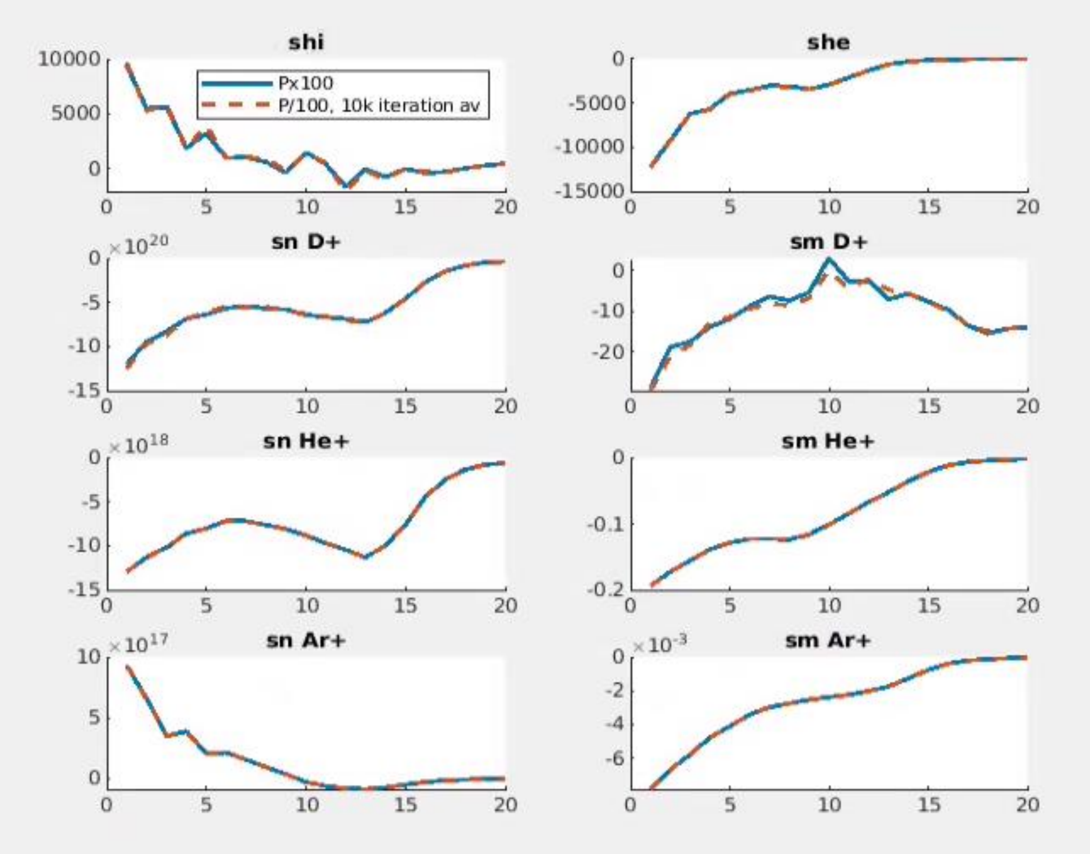
- Residuals and plasma time traces stagnate to statistical steady state





Error in EIRENE (e.g. source rescaling)?

- Compared 1 EIRENE call with 130M particles to average of 13k over 10k iterations on fixed plasma BG



→ seems OK

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