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Averaging schemes for speedup and error assessment of coupled FV-MC codes

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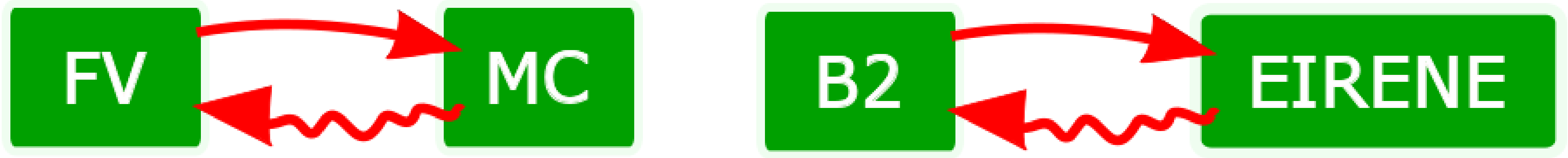
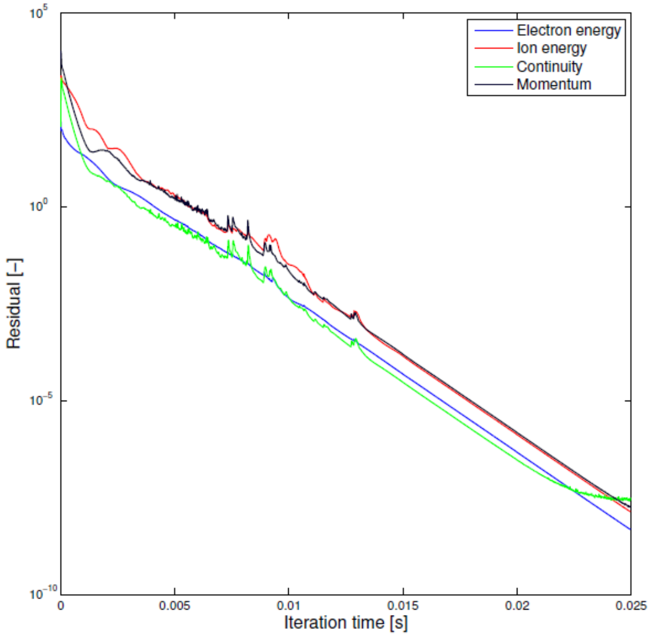
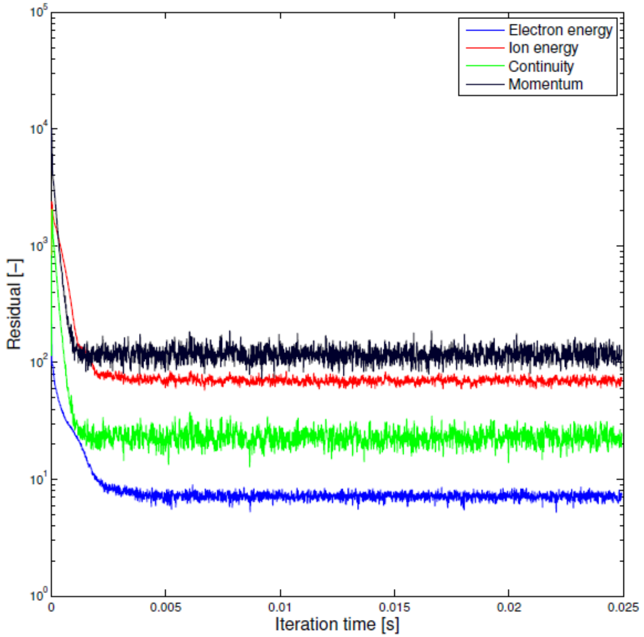
Convergence of coupled FV-MC codes?

Most plasma edge codes: fluid-kinetic code coupling







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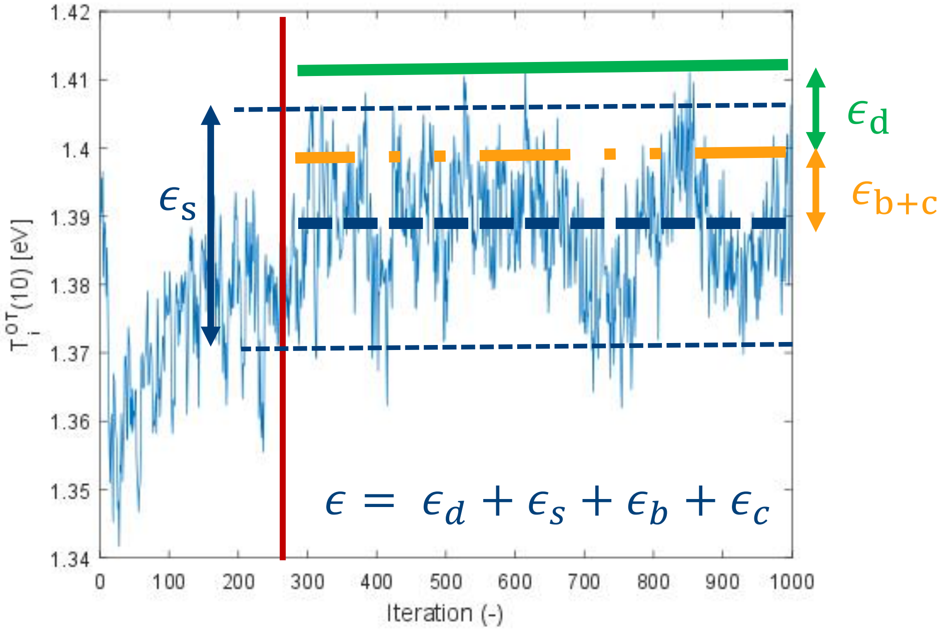
Numerical errors in coupled FV-MC systems

[K. Ghoos et al., JCP ***322*** *(2016) 162]*

Different error contributions

- Statistical error ϵ_s — Finite P
- Finite sampling bias ϵ_b — Finite P
- Convergence error ϵ_c — Non-zero res.
- Discretization error ϵ_d — Finite *h*



Post-processing averaging improves accuracy

Random noise procedure (RN)

- Provides smallest errors **(ε_s ↓)**
- Convergence and bias together

$$\varepsilon = A_d h^p + \frac{A_s^{RN}}{\sqrt{P I_{av}}} + \frac{A_{bc}^{RN}}{P}$$

P: # of MC particles per iteration,
I: # of iterations,
h: char. grid size

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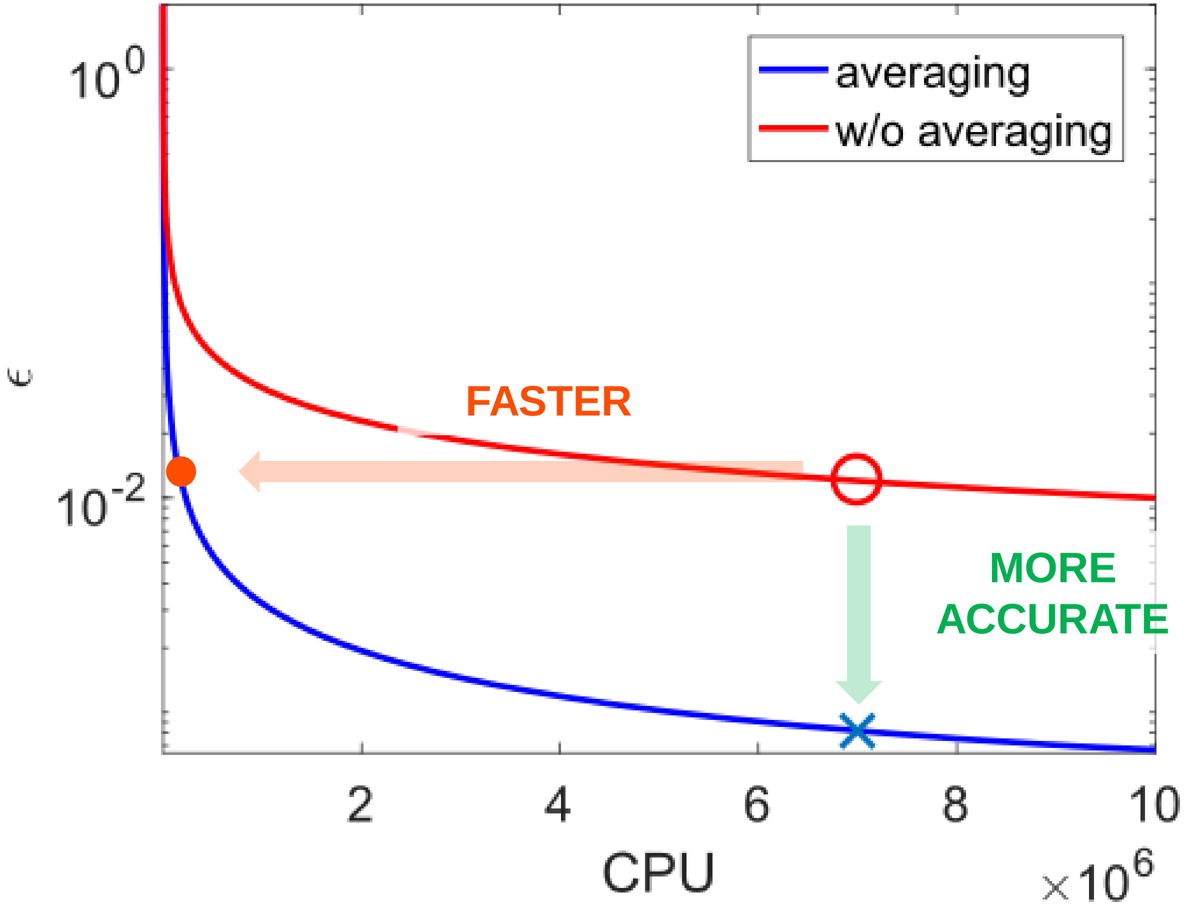
Averaging: faster, or more accurate



Why does it work?

- In practical situations, statistical error usually dominant over bias/convergence error
- Reducing this error requires a large number of particles, *but not necessarily from a single iteration*
- By averaging over many iterations with few particles per iteration:
  - fewer particles 'wasted' in transient phase
  - price to pay: slightly higher bias error

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Final procedure for error estimation

1. Estimate **statistical** error
   - Reduce this error by averaging over iterations
   - Note: averaging only in steady state (visual inspection of time traces)

$$\epsilon_s \approx \frac{3\sigma}{\sqrt{PI_{av}/T}} \qquad \sigma \approx s = \sqrt{\frac{1}{R-1}\sum_{r=1}^{R}(\phi_r - \bar{\phi})^2}$$

$$\bar{\phi}$$

Averaged solution

2. Estimate finite sampling **bias** by comparing two solutions on same grid, with different number of MC particles

$$\epsilon_{b,P} \approx \alpha \frac{\bar{\phi}_P - \bar{\phi}_{\alpha P}}{1-\alpha}$$

$$\phi_\infty \approx \bar{\phi}_P + \epsilon_{b,P}$$

Bias-corrected solution

3. Estimate **discretization** error by comparing solutions on successively finer grids (3 grid levels)
   - ⇒ Note that a total of **6** simulations is required in order to estimate all errors
   - ⇒ Can be reduced to **4** if order of the (spatial) discretization scheme is known

$$\epsilon_{d,h} \approx \frac{\phi_{\infty,h} - \phi_{\infty,2h}}{2^p - 1} \qquad p = \frac{\log \frac{\phi_{\infty,2h} - \phi_{\infty,4h}}{\phi_{\infty,h} - \phi_{\infty,2h}}}{\log 2}$$

$$\phi_{exact} \approx \phi_{\infty,h} + \epsilon_{d,h}$$

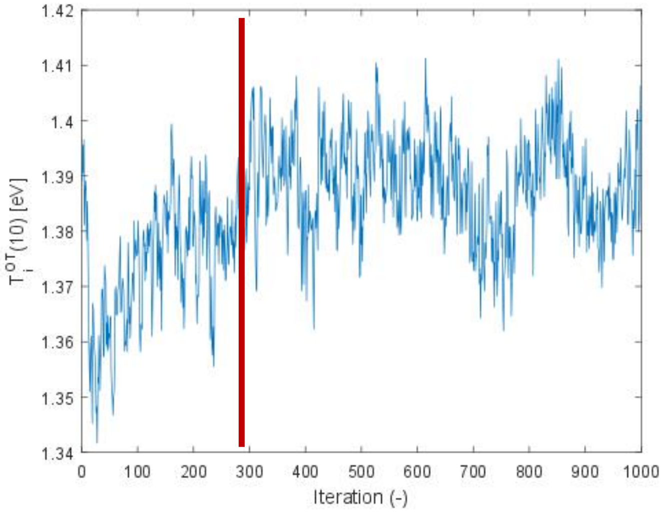
"Exact" solution

Simulation procedure for RN

Batch 1 500 iter	…	Batch x 500 iter	Batch x+1 500 iter	…	Batch n-1 500 iter	Batch n 500 iter
$\bar{\phi}_1, \overline{\phi^2}_1, \bar{S}_1$		$\bar{\phi}_x, \overline{\phi^2}_x, \bar{S}_x$	$\bar{\phi}_{x+1}, \overline{\phi^2}_{x+1}, \bar{S}_{x+1}$		$\bar{\phi}_{n-1}, \overline{\phi^2}_{n-1}, \bar{S}_{n-1}$	$\bar{\phi}_n, \overline{\phi^2}_n, \bar{S}_n$

Transient phase

Statistically steady regime
(Running) averaging phase



Final solution and statistical error

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Implementation in SOLPS-ITER

1. **Case setup**: fully random seed for EIRENE particles (no seed number)

2. **Monitor transient phase**: check time traces of selected quantities ($n_e, T_e, T_i,$ ... at OMP, IMP, targets) averaged over *ntim_batch* iterations in **b2batch.nc**
→ less noisy quantities than instantaneous ones
Full 2D fields also possible

3. **Averaging phase:** started/continued with switch, update running average of state ($\overline{n_e}$, $\overline{T_e}$,..,$\overline{S_n}$, $\overline{S_{mom}}$,..) and ($\overline{n_e^2}$, $\overline{T_e^2}$,..,$\overline{S_n^2}$, $\overline{S_{mom}^2}$,..) → <u>does not interfere with simulation</u>! **b2fstate** instantaneous noisy state, **b2favere** running average

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Implementation in SOLPS-ITER

4. **Obtain final solution:** 2 timesteps reading state from **b2favere** (via switch), no update in plasma state, only evaluate fluxes etc. based on averaged quantities and sources + high number of particles to get low statistical error on EIRENE quantities

5. **Statistical error assessment with b2ye:** based on batch averages from **b2batch.nc,** calculates standard deviation and correlation time

$$\epsilon_s \approx \frac{\sigma}{\sqrt{PI_{av}/T}} \qquad \sigma \approx s = \sqrt{\frac{1}{R-1}\sum_{r=1}^{R}(\phi_r - \bar{\phi})^2}$$

Extra: convergence check on residuals with **res_av** script → performs step 4 of the procedure for running averaged states saved every *ntim_run* iterations

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- Baelmans, M., Börner, P., Ghoos, K., Samaey, G. (2016). Efficient code simulation strategies for B2-EIRENE. Nuclear Materials and Energy, (12), 856-863.
- K. Ghoos, P. Börner, W. Dekeyser, A. Kukushkin, and M. Baelmans, Grid resolution study for B2-EIRENE simulation of partially detached ITER divertor plasma, Nuclear Fusion, vol. 59, p. 026001, 2019.

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