Comparison of different iterative schemes in B2 for full-scale ITER cases. Task WPCD-SOLPS-OPT

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Initial state

- Common way of doing B2-EIRENE ITER simulations: with internal iterations
- Problem: time-step is restricted to $\Delta t =$1e-7..1e-6 sec $\Rightarrow$ $n\times$month for one simulation
- W/o internal iterations: time-step $\Delta t =$1e-4...1e-3 sec
- Problem: lower accuracy
  - "0-order" effect - particle balance
  - Bad parallel momentum balance, especially for impurities
- Large error in the global particle balance can drive the solution into completely wrong direction
- **Goal: to achieve (at least) same accuracy of B2-EIRENE as with internal iterations but with large time-step**

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How to increase the accuracy with large Δt ?

- Simplest method is the 0D correction: re-scale the whole 2D density profile to formally fulfill the particle balance
- Does not work: long period oscillations, no stationary solution
- 0D does not work, try to solve the continuity equations: do one full internal iteration, then do extra iterations to relax the continuity equations only - “continuity iterations”
- Works! Robust with Δt up to 1e-4 sec
- Pitfall: degradation of accuracy of other equations
- Especially the momentum balance suffers
- see report `www.eirene.de/Juel-4371-kotov.pdf`
- Next method to try: iterate *coupled* particle and momentum balance after one full iteration - “incomplete iterations”

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“Incomplete iterations”

$\phi^0 := \{n_\alpha^0, u_\alpha^0, T_e^0, T_i^0\} = \phi_{k-1}^m$

for $j = 0 : m - 1$ **do**

1. source terms, coefficients and BC
2. momentum, $\forall\alpha$: $u_\alpha^{j+1/3} = u_\alpha^j + r\xi$
3. total momentum, $\sum_\alpha$: $u_\alpha^{j+2/3} = u_\alpha^{j+1/3} + r\xi$
4. continuity, $\forall\alpha$: $n_\alpha^{j+1} = n_\alpha^j + r\xi$, $u_\alpha^{j+1} = u_\alpha^{j+2/3} - rC\frac{\partial\xi}{\partial x}$

if $j == 0$ **then**

5. electron energy: $T_e^{j+1/2} = T_e^j + r\xi$
6. ion energy: $T_i^{j+1/2} = T_i^j + r\xi$
7. total en.: $T_e^{j+1} = T_e^{j+1/2} + r\xi$, $T_i^{j+1} = T_i^{j+1/2} + r\xi$

end if

end for

$\mathrm{M}(\phi_0)\,\xi = S(\phi_0) - \mathrm{M}(\phi_0)\,\psi_0 = R, \quad \psi = n_\alpha$ or u_α or T_e or T_i

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Implementation and tests

- Experience from implementation of continuity iterations: a hidden mistake was found in B2CCON which could affect the convergence rate
- Hence, B2CMOM was completely re-written $\rightarrow$ B2CMOMVK
- Test cases:

  Single ion **#2013vk1**, *D*, P_{SOL}=38 MW, Γ_{puff}=1.2e22 s^{-1}, p_{PFR}=3 Pa, f_{rad}=0.14

  Multi-ion **#1568vk4**, F57, $D + He + C$, P_{SOL}=80 MW, Γ_{puff}=1.2e22 s^{-1}, p_{PFR}=2 Pa, weak level of detachment, weak $||$ momentum losses, f_{rad}=0.47

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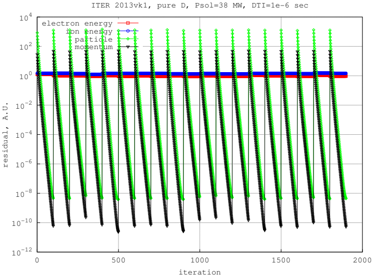
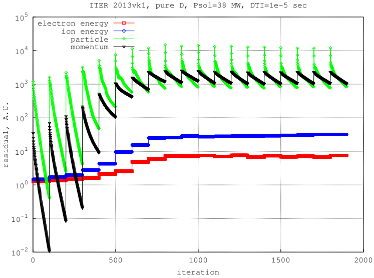
"Convergence" vs "numerical instability"

- All cases started from the same stationary solution
- 20 time-iterations, *m*=1+99

An example for "iterations converge"



An example for "numerical instability"



Incomplete iterations, single-ion test #2013vk1

- Δt=1e-6 sec $\Rightarrow$ converge
- Δt=1e-5 sec $\Rightarrow$ instability
- Δt=1e-4 sec $\Rightarrow$ instability
- Linearized momentum equation $u = fixed$, $v = fixed$
- Δt=1e-6 sec $\Rightarrow$ converge
- Δt=1e-5 sec $\Rightarrow$ instability
- Δt=1e-4 sec $\Rightarrow$ instability
- Linearized momentum equation
  $u = fixed$, $v = fixed$, $n = fixed$
- Δt=1e-6 sec $\Rightarrow$ converge
- Δt=1e-5 sec $\Rightarrow$ instability
- Δt=1e-4 sec $\Rightarrow$ instability

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Dual time-step approach

- Δt_m for momentum equation, Δt for all other equations
- Time-scale of the parallel momentum balance could be short, thus $\Delta t_m << \Delta t$
- Single-ion #2013vk1
- $\Delta t_m =$1e-7 sec, $\Delta t =$1e-5 sec $\Rightarrow$ converge (surprised !?)
- $\Delta t_m =$1e-7 sec, $\Delta t =$1e-4 sec $\Rightarrow$ converge
- $\Delta t_m =$1e-7 sec, $\Delta t =$1e-4 sec, $m =$1+499 $\Rightarrow$ converge
- $\Delta t_m =$1e-7 sec, $\Delta t =$1e-4 sec, $m =$1+499, Γ_{puff}=1e23 s^{-1} (detached divertor) $\Rightarrow$ converge (!!!)

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Multi-ion test #1568vk4

- Friction between ions $\sum_\beta k_\beta n n_\beta \left(u_{||}^\beta - u_{||}\right)$ is switched off
- Relaxation of the total momentum is switched off
- $\Delta t = \Delta t_m =$1e-6 sec $\Rightarrow$ converge
- $\Delta t = \Delta t_m =$1e-5 sec $\Rightarrow$ instability
- $\Delta t_m =$1e-7 sec, $\Delta t =$1e-5 sec $\Rightarrow$ instability (as usual ☹)
- Same result with B2CMOMVK and B2CMOM

- **In general, incomplete iterations lead to instability with large** Δt ($>$1e-6 sec), same as full internal iterations

Improved source-term linearization

$$S = \bar{S} + \hat{S}\psi$$

- Stability analysis of linearized equations with fixed transport part wrt. small perturbations

$$\frac{\partial n_\alpha}{\partial t} = S^n_\alpha + F^n_\alpha = \bar{S}^n_\alpha + \hat{S}^n_\alpha n_\alpha + F^n_\alpha$$

$$\frac{\partial\left(m_\alpha n_\alpha u_\alpha\right)}{\partial t} = S^u_\alpha + F^u_\alpha = \bar{S}^u_\alpha + \hat{S}^u_\alpha u_\alpha + F^u_\alpha$$

$$\frac{\partial\left(\frac{3}{2} T_e \sum_\alpha Z_\alpha n_\alpha\right)}{\partial t} = S^E_e + F^E_e = S^E_e + \hat{S}^E_e T_e + F^E_e$$

$$\frac{\partial\left(\frac{3}{2} T_i \sum_\alpha n_\alpha + \frac{1}{2} \sum_\alpha m_\alpha n_\alpha u^2_\alpha\right)}{\partial t} = S^E_i + F^E_i = \bar{S}^E_i + \hat{S}^E_i T_i + F^E_i$$

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Source-term linearization, continued

$$\hat{S}_\alpha^n \leq 0$$

$$\hat{S}_\alpha^u - m_\alpha \left(S_\alpha^n + F_\alpha^n\right) = \hat{S}_\alpha^u - m_\alpha \frac{\partial n_\alpha}{\partial t} \leq 0$$

$$\hat{S}_e^E - \frac{3}{2} \sum_\alpha Z_\alpha \left(S_\alpha^n + F_\alpha^n\right) = \hat{S}_e^E - \frac{3}{2} \frac{\partial n_e}{\partial t} \leq 0$$

$$\hat{S}_i^E - \frac{3}{2} \sum_\alpha \left(S_\alpha^n + F_\alpha^n\right) = \hat{S}_i^E - \frac{3}{2} \frac{\partial n_i}{\partial t} \leq 0$$

- Source linearization of B2 ensures $\hat{S} < 0$
- Guarantees fulfillment of the above conditions only if $S^n > 0$ ($F^n = 0$), that is, no volume recombination
- Stricter linearization was implemented and tested
- **No improvement detected**

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Robbins-Monro iteration

- Look for solution x^* of $M(x) = 0$, $M(x) = \overline{Y(x)}$ where $Y(x)$ is a random function
- [H. Robbins, S. Monro, 1951]

$$x_{n+1} = x_n - a_n y_n, \quad y_n = \text{sample of } Y(x_n)$$

converges to x^* if (sufficient condition)

$$a_n > 0 \quad \text{and} \quad \sum_{n=1}^{\infty} a_n \to \infty \quad \text{and} \quad \sum_{n=1}^{\infty} a_n^2 < \infty$$

- E.g.

$$a_n = \frac{1}{n^\alpha}, \quad 0.5 < \alpha \leq 1$$

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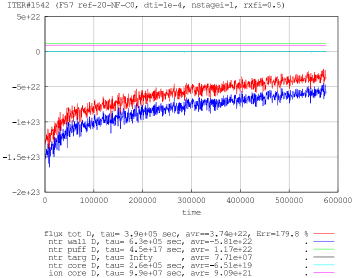
Robbins-Monro, continued

- Implementation in B2

$$r_k = \frac{r_0}{(k+1)^\alpha}$$

r is the relaxation parameter
k is the index of time-iteration



- Heuristic extension of Robbins-Monro algorithm
  - without formal proof
- Test: #1568vk4, started from high-density case #1542vk4, $\alpha = 0.6$, Δt=10 sec - fixed point solution
- **Stable but very slow convergence**

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Summary and outlook

- Robbins-Monro iterations may converge but too slow for practical applications
- Incomplete iterations lead to instability with large time-steps (Δt >1e-6 sec)
  - Approach with decreased Δt for momentum balance worked for single-ion test, but did not work for multi-ion test, even w/o friction term
- Improved source linearization does not help
- Hypothesis: Patankar's SIMPLE pressure correction ($u_\alpha^{j+1} = u_\alpha^{j+2/3} - rC\frac{\partial \xi}{\partial x}$) might hinder convergence (???)
- **Proposal: to try monolithic coupling of the particle and momentum balance** instead

$$\begin{bmatrix} P_n & Q_n \\ P_u & Q_u \end{bmatrix} \begin{bmatrix} n \\ u \end{bmatrix} = \begin{bmatrix} S_u \\ S_n \end{bmatrix} \Rightarrow \begin{bmatrix} n \\ u \end{bmatrix}$$

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Concluding remarks 1

- The ultimate goal was to achieve same accuracy of B2-EIRENE as with internal iterations but keeping large time-step (Δt =1e-4..1e-3)
- No universal solution, two robust methods
- "Continuity iterations" - extra iterations for continuity (pressure correction) equations only

  Drawback: accuracy of other equations degrades
- Increase of the number of MC particles by a factor of $\gtrsim$100

  Drawbacks: requires 100s-1000s of CPUs,
  does not always help for impurities

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Concluding remarks 2

- Observation: normally good convergence for single-ion plasmas even w/o internal iterations
- Two methods are found to work for single-ion plasma and failed for multi-ion (or I screwed it up):
  - Time-averaging of source terms
  - Reduced time-step for momentum balance
- For ITER, numerically it can be more efficient to remove He from B2-EIRENE simulations and to model it during post-processing as trace-impurity

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Backup

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Parallel momentum balance equation

$$\frac{1}{\sqrt{g}}\frac{\partial}{\partial x}\frac{\sqrt{g}}{h_x}\left(mnuu_{||} - \frac{2}{3}\eta_x \frac{1}{1+\left|\frac{\frac{2}{3}\eta_x\frac{\partial u_{||}}{\partial x}}{f_{lim}b_x n T_i}\right|}\frac{1}{h_x}\frac{\partial u_{||}}{\partial x}\right) +$$

$$+\frac{1}{\sqrt{g}}\frac{\partial}{\partial y}\frac{\sqrt{g}}{h_y}\left(mnvu_{||} - \eta_y\frac{1}{h_y}\frac{\partial u_{||}}{\partial y}\right) = -\frac{b_x}{h_x}\frac{\partial p}{\partial x} +$$

$$+\frac{b_x}{h_x}\left[-\frac{Zn}{n_e}\frac{\partial p_e}{\partial x} + c_e\left(\frac{Z}{Z_{eff}} - 1\right)Zn\frac{\partial T_e}{\partial x} + c_i\left(\frac{Z}{Z_{eff}} - 1\right)Zn\frac{\partial T_i}{\partial x}\right] +$$

$$+S_{mu_{||}} + \sum_\beta k_\beta n n_\beta\left(u_{||}^\beta - u_{||}\right) - \frac{\partial mnu_{||}}{\partial t}$$

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