KU LEUVEN

TSVV3 – Task 7: Status and plans EBC code

W. Dekeyser, P. Tamain, G. Brethes, J. Parker, M. Wiesenberger, A. Stegmeir, J. Fausty, G. Giorgiani, TSVV3 team

Motivation

- Why HDG-approach?
	- o Allows detailed geometrical description of the wall
	- o Grid flexibility
	- o High order, p-adaptivity
	- o Highly parallelizable
	- o Cheaper than standard implicit FEM
- Drawbacks HDG-approach?
	- \circ High order \Rightarrow badly conditioned matrices

2D interchange model

• Targeted first model

$$
\partial_t n + \nabla \cdot (n(\boldsymbol{u}_E - T_e \boldsymbol{K}) - D_\perp \nabla_\perp n) = S_n
$$

$$
\partial_t n_n + \nabla \cdot \left(\frac{n_{n,eq}}{n} (n\boldsymbol{u}_E + p_i \boldsymbol{K}) - \frac{p_i}{B} \boldsymbol{b} \times \nabla_\perp \left(\frac{n_{n,eq}}{n}\right) - \frac{1}{n(K_{cx} + K_i)} \nabla_\perp (T_i n_n) \right) = S_{n_n}
$$

$$
\partial_t p_e + \frac{5}{3} \nabla \cdot \left(p_e \boldsymbol{u}_E - \frac{p_e^2}{n} \boldsymbol{K} - \frac{p_e}{n} D_\perp \nabla_\perp n\right) - \frac{2}{3} \nabla \cdot (\chi_{\perp,e} n \nabla_\perp T_e) = S_{p_e}
$$

$$
\partial_t p_i + \frac{5}{3} \nabla \cdot \left(p_i \boldsymbol{u}_E + \frac{p_i^2}{n} \boldsymbol{K} - \frac{p_i}{n} D_\perp \nabla_\perp n\right) - \frac{2}{3} \nabla \cdot (\chi_{\perp,i} n \nabla_\perp T_i) = S_{p_i}
$$

$$
\partial_t W + \nabla \cdot (W(\boldsymbol{u}_E + T_i \boldsymbol{K}) - \nu \nabla_\perp W) + \nabla \cdot ((p_i + p_e + p_n) \boldsymbol{K}) = S_W
$$

with

$$
W = \nabla \cdot \left(\frac{\nabla_{\perp} \phi}{B^2} + \frac{\nabla_{\perp} p_i}{B^2}\right)
$$

$$
\mathbf{u}_E = \frac{\mathbf{b} \times \nabla \phi}{B}, \quad \mathbf{K} = 2\frac{\mathbf{b} \times \nabla \ln B}{B}, \quad n_{e,eq} = \frac{n_n K_{cx} + nK_r}{K_{cx} + K_i}
$$

2D interchange model

• Targeted first model

$$
\partial_t n + \nabla \cdot \left(n(\boldsymbol{u}_E - T_e \boldsymbol{K}) - D_\perp \nabla_\perp n \right) = S_n
$$

$$
\partial_t n_n + \nabla \cdot \left(\frac{n_{n,eq}}{n} \left(n\boldsymbol{u}_E + p_i \boldsymbol{K} \right) - \frac{p_i}{B} \boldsymbol{b} \times \nabla_\perp \left(\frac{n_{n,eq}}{n} \right) - \frac{1}{n(K_{cx} + K_i)} \nabla_\perp (T_i n_n) \right) = S_{n_n}
$$

$$
\partial_t p_e + \frac{5}{3} \nabla \cdot \left(p_e \boldsymbol{u}_E - \frac{p_e^2}{n} \boldsymbol{K} - \frac{p_e}{n} D_\perp \nabla_\perp n \right) - \frac{2}{3} \nabla \cdot (\chi_{\perp,e} n \nabla_\perp T_e) = S_{p_e}
$$

$$
\partial_t p_i + \frac{5}{3} \nabla \cdot \left(p_i \boldsymbol{u}_E + \frac{p_i^2}{n} \boldsymbol{K} - \frac{p_i}{n} D_\perp \nabla_\perp n \right) - \frac{2}{3} \nabla \cdot (\chi_{\perp,i} n \nabla_\perp T_i) = S_{p_i}
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$$
\partial_t W + \nabla \cdot \left(W \left(\boldsymbol{u}_E + T_i \boldsymbol{K} \right) - \nu \nabla_\perp W \right) + \nabla \cdot \left((p_i + p_e + p_n) \boldsymbol{K} \right) = S_W
$$

 s set of coupled advection-diffusion-reaction equations for $U = \{U_1,...,U_5\}^T = \{n,n_{\rm n},p_{\rm e},p_{\rm i},W\}^T$

$$
\partial_t \boldsymbol{U} + \boldsymbol{\nabla} \cdot (\boldsymbol{C}(\boldsymbol{U}) + \boldsymbol{K}(\boldsymbol{U})\boldsymbol{q}) = \boldsymbol{S}(\boldsymbol{U}), \qquad \boldsymbol{q} + \nabla_{\perp}\boldsymbol{U} = 0
$$

Solution with HDG approach

- Implementation: models & operators
	- o Model: build matrix contributions at the element level
	- o Operator: construct contributions from individual terms in the model
	- o Flexibility to implement different models and discretization options

$$
\begin{bmatrix} A_{uu} & A_{uq} & A_{ul} \\ A_{qu} & A_{qq} & A_{ql} \\ A_{lu} & A_{lq} & A_{ll} \end{bmatrix} \begin{bmatrix} u \\ q \\ \lambda \end{bmatrix} = \begin{bmatrix} B_u \\ B_q \\ B_l \end{bmatrix} \begin{array}{c} \text{model eq.} \\ q + \nabla u = 0 \\ \text{trace eq.} \end{array}
$$

Breakdown into operators

• Diffusion operator: implicit

$$
\boldsymbol{K}(\boldsymbol{U})\boldsymbol{q} = \begin{bmatrix} \kappa_{1,1}(\boldsymbol{U}) & \kappa_{1,2}(\boldsymbol{U}) & \ldots & \kappa_{1,\text{nEq}}(\boldsymbol{U}) \\ \ldots & \ldots & \ldots & \ldots \\ \kappa_{\text{nEq},1}(\boldsymbol{U}) & \kappa_{\text{nEq},2}(\boldsymbol{U}) & \ldots & \kappa_{\text{nEq},\text{nEq}}(\boldsymbol{U}) \end{bmatrix} \begin{bmatrix} \boldsymbol{q}_1 \\ \ldots \\ \boldsymbol{q}_{\text{nEq}} \end{bmatrix}
$$

• For the 2D interchange model, with $\mathbf{U} = \{\mathbf{U}_1, ..., \mathbf{U}_5\}^T = \{n, n_{\rm n}, p_{\rm e}, p_{\rm i}, W\}^T$

$$
\boldsymbol{K}(\boldsymbol{U}) = \begin{bmatrix} D_{\perp} & 0 & 0 & 0 & 0 \\ 0 & \frac{\boldsymbol{U}_{4}}{\boldsymbol{U}_{1}(K_{cx} + K_{i})} & 0 & \frac{\boldsymbol{U}_{2}}{\boldsymbol{U}_{1}(K_{cx} + K_{i})} & 0 \\ \frac{5}{2}\boldsymbol{U}_{3}D_{\perp} & 0 & \chi_{\perp,e}\boldsymbol{U}_{1} & 0 & 0 \\ 0 & 0 & 0 & \chi_{\perp,i}\boldsymbol{U}_{1} & 0 \\ 0 & 0 & 0 & 0 & \nu \end{bmatrix}
$$

 t ime lagging for the diffusion matrix: evaluate at U^n

Breakdown into operators

• Advection operator: explicit, upwind

$$
C(\boldsymbol{U}) = \begin{bmatrix} \boldsymbol{U}_1 \mathbf{v}_1 \\ \dots \\ \boldsymbol{U}_{n \to q} \mathbf{v}_{n \to q} \end{bmatrix}
$$

• Reaction (implicit, time-lagging) and source (explicit) operators

$$
S(U) = \begin{bmatrix} R_{1,1}(U) & R_{1,2}(U) & \dots & R_{1,\text{nEq}}(U) \\ \dots & \dots & \dots & \dots \\ R_{nEq,1}(U) & R_{nEq,2}(U) & \dots & R_{nEq,\text{nEq}}(U) \end{bmatrix} \begin{bmatrix} U_1 \\ \dots \\ U_{nEq} \end{bmatrix}
$$

$$
S(U) = \begin{bmatrix} f_1(U) \\ \dots \\ f_{nEq}(U) \end{bmatrix}
$$

Simple advection-diffusion-reaction model

• Single advection-diffusion-reaction equation with linear analytical solution $\bar{u} = 0.1x + 0.2y + 0.3$

$$
\partial_t u + \nabla \cdot (u\mathbf{v} - D\nabla u) = S - Ru \quad \text{on} \quad \Omega
$$

$$
u = \bar{u}|_{\partial \Omega} \qquad \text{on} \quad \partial \Omega
$$

Solenoidal velocity field $\boldsymbol{v} = \{-0.2, 0.1\}^T$; constant, isotropic diffusion tensor D Source chosen to have constant R and $S = R\bar{u}$

• *N* coupled equations, linear analytical solutions $\bar{u}_i = i\bar{u}$

$$
\partial_t u_i + \nabla \cdot \left(u_i v - \sum_{j=1,N} D_{i,j} \nabla u_j \right) = S_i - \sum_{j=1,N} R_{i,j} u_j \quad \text{on} \quad \Omega
$$

$$
u_i = \bar{u}_i \big|_{\partial \Omega} \qquad \text{on} \quad \partial \Omega
$$

Same velocity field; isotropic diffusion tensor with $D_{i,j} = \frac{i}{jN} D$; source rate $R_{i,j} = \frac{i}{jN} R$

Simple advection-diffusion-reaction model

Solution (-) Error (-)

Diffusion equation, arbitrary element order

Time (in)dependent equations

• Additional "diffusion-reaction" equation for potential, time-independent

$$
\partial_t n + \nabla \cdot \left(n(u_E - T_e K) - D_\perp \nabla_\perp n \right) = S_n
$$

$$
\partial_t n_n + \nabla \cdot \left(\frac{n_{n,eq}}{n} \left(n u_E + p_i K \right) - \frac{p_i}{B} b \times \nabla_\perp \left(\frac{n_{n,eq}}{n} \right) - \frac{1}{n(K_{cx} + K_i)} \nabla_\perp (T_i n_n) \right) = S_{n_n}
$$

$$
\partial_t p_e + \frac{5}{3} \nabla \cdot \left(p_e u_E - \frac{p_e^2}{n} K - \frac{p_e}{n} D_\perp \nabla_\perp n \right) - \frac{2}{3} \nabla \cdot (\chi_{\perp,e} n \nabla_\perp T_e) = S_{p_e}
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$$
\partial_t p_i + \frac{5}{3} \nabla \cdot \left(p_i u_E + \frac{p_i^2}{n} K - \frac{p_i}{n} D_\perp \nabla_\perp n \right) - \frac{2}{3} \nabla \cdot (\chi_{\perp,i} n \nabla_\perp T_i) = S_{p_i}
$$

$$
\partial_t W + \nabla \cdot \left(W \left(u_E + T_i K \right) - \nu \nabla_\perp W \right) + \nabla \cdot \left((p_i + p_e + p_n) K \right) = S_W
$$

$$
-\nabla \cdot \left(\frac{\nabla_\perp \phi}{B^2} + \frac{\nabla_\perp p_i}{B^2} \right) = -W
$$

 s set of coupled equations for $\bm{U} = \{\bm{U}_1,...,\bm{U}_5,\bm{U}_6\}^T = \{n,n_\mathrm{n},p_\mathrm{e},p_\mathrm{i},W,\phi\}^T$

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Next steps

• Implement toy model

$$
\partial_t n + \nabla \cdot (n \mathbf{u}_E - D_\perp \nabla_\perp n) = 0
$$

$$
n - \nabla \cdot \left(\frac{\nabla_\perp \phi}{B}\right) = 0
$$

• Implement full 2D interchange model