

SOLEGE-HDG: a novel unstructured approach for transport simulations in tokamak-relevant conditions

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Contributors

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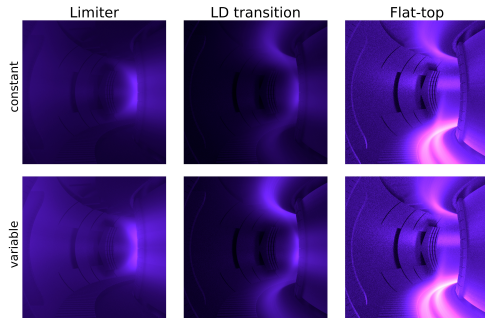


Figure: Visible light reconstruction of WEST plasma from outputs of SolEdge-HDG (courtesy I. Kudashev).

Motivation for transport mean field codes



Figure: Visible light imaging of the inside of tokamak WEST

Objectives for Soledge-HDG modelling

- evaluate particle and heat fluxes towards plasma-facing components
- construct reasonable density and temperature profiles throughout the plasma
- use appropriate sources for particle content and heat deposition inside the plasma
- model plasma/wall interactions

Physical model - Braginskii equations without drifts

$$\mathbf{U} = [n, nu, nE_i, nE_e]^T \quad \mathbf{Q} = \nabla \mathbf{U}.$$

$$\begin{cases} \partial_t \mathbf{U} + \nabla \cdot \mathbf{F} - \nabla \cdot (D\mathbf{Q}) - \nabla \cdot \mathbf{F}_t + \mathbf{f}_{E\parallel} + \mathbf{f}_{EX} - \mathbf{g} = \mathbf{s} & \text{in } \Omega \times]0, T_f[\\ \mathbf{Q} - \nabla \mathbf{U} = \mathbf{0} & \text{in } \Omega \times]0, T_f[\\ \mathbf{U}(\mathbf{x}, 0) = \mathbf{U}_0 & \text{in } \Omega \end{cases}$$

$$\begin{aligned} \mathbf{F} &= \begin{bmatrix} nu \\ nu^2 + M(p_i + p_e) \\ (nE_i + Mp_i)u \\ (nE_e + Mp_e)u \end{bmatrix} \otimes \mathbf{b}^T, & \mathbf{F}_t &= \begin{bmatrix} 0 \\ 0 \\ k_{\parallel i} T_i^{5/2} \nabla_{\parallel} T_i \\ k_{\parallel e} T_e^{5/2} \nabla_{\parallel} T_e \end{bmatrix} \otimes \mathbf{b}^T, & \mathbf{f}_{E\parallel} &= Mu \nabla_{\parallel} p_e \begin{bmatrix} 0 \\ 0 \\ 1 \\ -1 \end{bmatrix}, \\ \mathbf{f}_{EX} &= \frac{n^2}{\tau_{ie}} \frac{T_e - T_i}{T_e^{3/2}} \begin{bmatrix} 0 \\ 0 \\ 1 \\ -1 \end{bmatrix}, & \mathbf{g} &= \begin{bmatrix} 0 \\ (p_i + p_e) \nabla \cdot \mathbf{b} \\ 0 \\ 0 \end{bmatrix} \end{aligned}$$

completed with Bohm boundary conditions, and especially

$$u(\mathbf{b} \cdot \mathbf{n}) \geq c_s$$

Choice of spatial discretization

Braginskii equations as a generalized, nonlinear advection-diffusion-reaction problem.

Discretization	Conservativity	Complex geometries	High-order accuracy	Structure
Finite-difference	✓	✓	✓	✓
Finite-volume	✓	✓	✓	✗
Finite-element	✗	✓	✓	✗
Spectral methods	✓	✗	✓	✓
Discontinuous Galerkin	✓	✓	✓	✗

Discontinuous Galerkin methods check all boxes, except for structure.

Discontinuous Galerkin - high-order finite elements

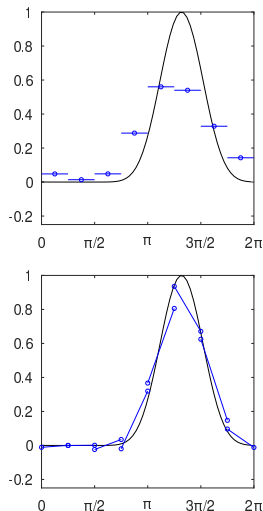
- simple advection problem in 1D

$$\begin{cases} \frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0 & \forall (x, t) \in [-\pi, \pi] \times [0, T] \\ u(x, t = 0) = [\sin(x/2)]^{10} \end{cases}$$

- Weak formulation of nonlinear advection problem

$$\frac{\partial}{\partial t}(u, v)_{\Omega} + \langle (\hat{u} - u) \cdot n, v \rangle_{\partial\Omega} - (u, v')_{\Omega} = 0$$

- Local polynomial, piecewise continuous expansion



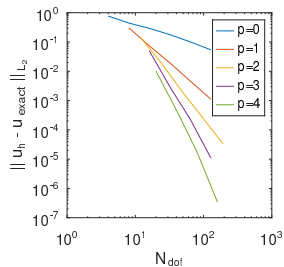
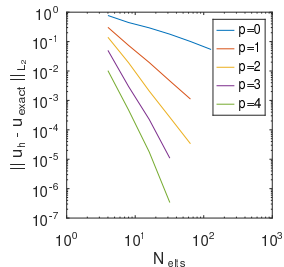
Figures on the right: comparison between exact solution (black) and numerical solution using approximation of order $p = 0$ (top), $p = 1$ (bottom).

Discontinuous Galerkin methods - high-order discretization

- Weak formulation of nonlinear advection problem

$$\frac{\partial}{\partial t}(u, v)_{\Omega} + \langle (\hat{f} - f) \cdot n, v \rangle_{\partial\Omega} - (f, v')_{\Omega} = 0$$

- time-step sufficiently small to eliminate time discretization errors,
- local polynomial expansion on control volume of order p ,
- convergence of error at order $p + 1$
- clear advantage on number of degrees of freedom using high-order approximations.



Discontinuous Galerkin methods - weak formulation

- weak formulation of nonlinear advection problem

$$\frac{\partial}{\partial t}(u, v)_{\Omega} + \langle (\hat{f} - f) \cdot n, v \rangle_{\partial\Omega} - (f, v')_{\Omega} = 0$$

- local polynomial, piecewise continuous expansion
- generalizations to 2D and 3D using Fekete points and orthogonal polynomial bases
- difficulty: defining the trace of $\hat{f}$ in a stable, consistent, accurate and efficient manner
- source of comfort: Discontinuous Galerkin methods are not new !

Reed W.H. and Hill T.R. Triangular mesh methods for the neutron transport equation. Los Alamos Scientific Lab., N.Mex. (USA), 1973
G. Karniadakis and S. Sherwin, Spectral/hp Element Methods for Computational Fluid Dynamics: Second Edition, Numerical Mathematics and Scientific Computation, 2013
D. A. Di Pietro and A. Ern, Mathematical Aspects of Discontinuous Galerkin Methods, Number 69 in Mathématiques & Applications, Springer, Berlin, 2011
J.S. Hesthaven and T. Warburton, 2008, Nodal Discontinuous Galerkin Methods: Algorithms, Analysis, and Applications. Springer Texts in Applied Mathematics 54, Springer Verlag, New York.

HDG: Hybridizable Discontinuous Galerkin

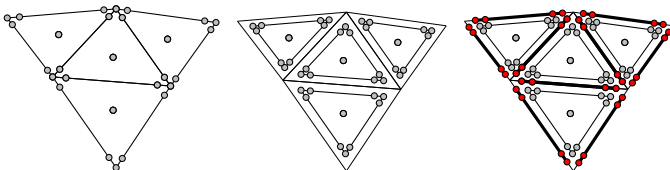


Figure: Representation of typical mesh with nodes corresponding to $p = 3$ for CG (left), DG (middle) and HDG (right) methods.

Treatment of trace values:

- Continuous Galerkin: imposes continuity of solutions on edges
- Discontinuous Galerkin: expresses edge values as function of elemental values and eliminates them
- Hybridizable Discontinuous Galerkin: relates edge values to elemental values but maintains them throughout the solution process

Hybridizable Discontinuous Galerkin - static condensation

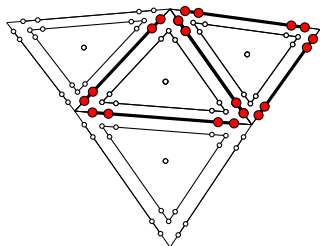


Figure: Representation of coupled edge values (in red) in the Schur complement.

Treatment of linear problem on in HDG discretization

- elimination of coupling between inner nodes and edge nodes through Gauss elimination,
- solution of a global problems on edge nodes only

$$\frac{N_{\text{dof,edges}}}{N_{\text{dof,total}}} \approx \frac{3}{p+2} \quad \text{in 2D}$$

- computation of inner node values through series of local, elemental problems

The physical basis

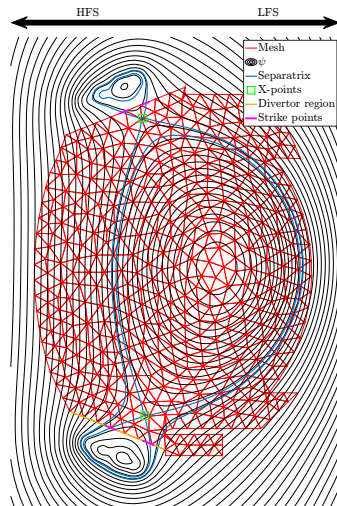
- two-dimensional mean-field code¹,
- bi-fluid model of transport with fluid neutrals,
- diffusive *ansatz* for averaged turbulent fluxes.

The numerical basis

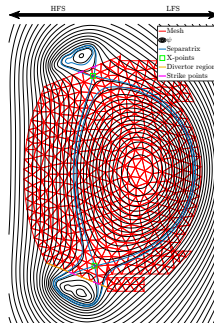
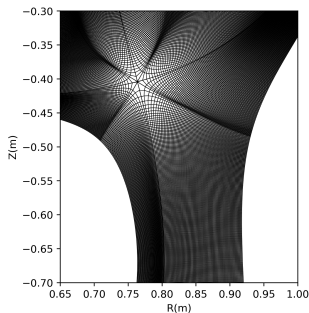
- simplicial meshes matching the boundary
- no account of magnetic configuration in meshes²

[1] G. Giorgiani *et al.*, A hybrid discontinuous Galerkin method for tokamak edge plasma simulations in global realistic geometry, J. Comp. Phys 2018

[2] G. Giorgiani *et al.*, A magnetic-field independent approach for strongly anisotropic equations arising plasma-edge transport simulations, Nuclear Materials and Energy 2019



Advantages of magnetic-independent, unstructured meshing

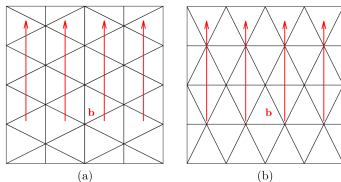


Magnetic-field-independent mesh: a defining characteristic

- easy fitting to wall geometry,
- no mesh singularities on X-points and magnetic axis,
- no long-range dependence of the mesh size,
- straightforward meshing with off-the-shelf, open-source software.

What is the price of not following magnetic surfaces ?

Test on 2D anisotropic diffusion with $k_{\parallel} \gg k_{\perp}$



A high-order non field-aligned approach for the discretization of strongly anisotropic diffusion operators in magnetic fusion
G. Giorgani *et al.*, Computer Physics Communications, 2020

Figure: Aligned mesh (left) and non-aligned mesh (right).

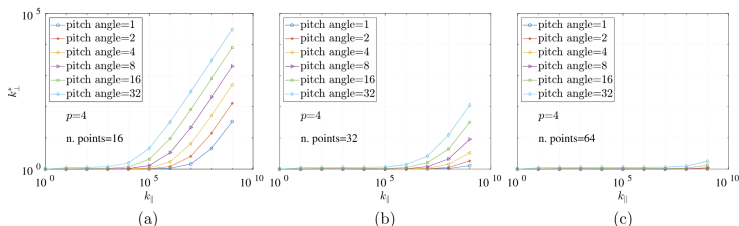


Figure: Effective perpendicular diffusivity as a function of parallel diffusivity.

SolEdge-HDG code: time-advancement scheme

- fully-implicit time discretization
- Newton-Raphson iterations
- pseudo-time advancement to steady state

Implicit time-advancement

$$U^{n+1} = U^n + \tau F(t^{n+1}, U^{n+1})$$

Newton-Raphson iterations with relaxation

$$U^{(p+1)} = U^{(p)} - \omega (J^{(p)})^{-1} [U^{(p)} - U^n - \tau F(t^{n+1}, U^{(p)})]$$

$$J^{(p)} = Id - \tau DF(t^{n+1}, U^{(p)})$$

Depending on the severity of the problem: 7 to 40 Newton iterations per pseudo-time-step.

SolEdge-HDG code

- written in Fortran
- direct inversion of Jacobian in Newton-Raphson iterations
- runs on multi-core workstations with OpenMP/MPI parallelization
- usual meshes with up to 500k elements with order 4 to 9 polynomial expansions
- typical runs last a few hours to several days

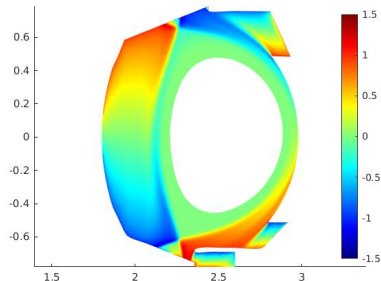
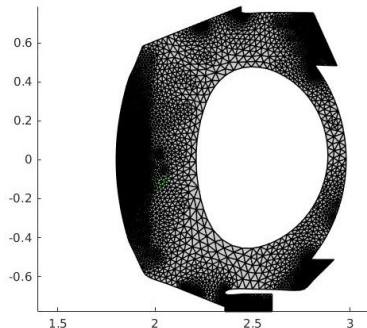


Figure: Mach number in the poloidal cross-section of WEST (G. Piraccini)

h -refinement in SolEdge-HDG

- Bohm boundary conditions require fine resolution close to walls,
- re-entrant corners are a challenge in all fields of numerical modelling,
- regular occurrence of divergence of Newton-Raphson iterations owing to local under-resolution,
- mesh design becomes a lengthy trial and error process,
- full-implicit time-stepping allows arbitrarily small elements without CFL restrictions.



Is computational time the only cost of modelling ?

Conforming h -refinement

- error "estimate" for solution at order p

$$\varepsilon_k = \|P_{\mathbb{P}_p^2(\Omega_k)} u_h - P_{\mathbb{P}_{p-1}^2(\Omega_k)} u_h\|$$

- oscillation detector identifies problematic elements for systematic refinement if $\varepsilon_k > \varepsilon_{\max}$
- optimization of local element diameter through *a posteriori* error estimate to predict element diameter on next mesh h^{n+1}

$$h^{(n+1)} = h^{(n)} \left(\frac{\varepsilon_{\text{target}}}{\varepsilon} \right)^{\frac{1}{p}}$$

- size information pushed back into meshing software for next mesh.

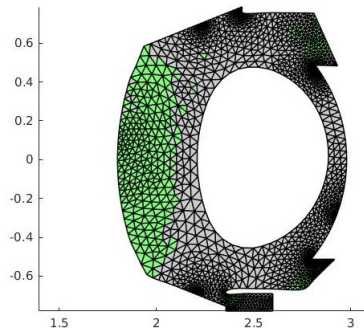
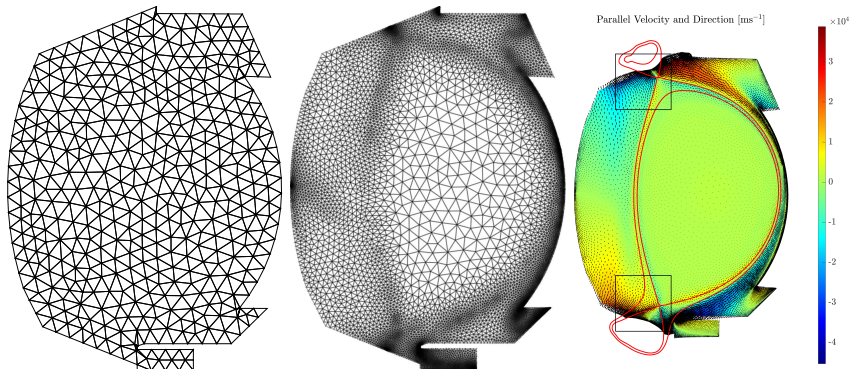


Figure: Identification of elements with excessive oscillations (G. Piraccini)

h -refinement



Adaptive h -refinement (PhD Giacomo Piraccini & post-doc Marcello Capasso)

Interest of adaptive mesh refinement

- automatic adaptation to solution
- reduction of N_{dof} : *lean* HPC (reduction of memory and computation)
- transfer of mesh design workload from user to computer

SolEdge-HDG - Time-varying magnetic configurations

Additional physics

- fluid neutral model
 - ▶ recycling
 - ▶ radiative energy losses
- input magnetic field for magnetic geometry and Ohmic heating

Modelling capabilities

- long-term simulations
- time-varying magnetic field
- transport modelling in 2D from ramp-up to ramp-down
- evaluation of power deposition on plasma-facing components during transients

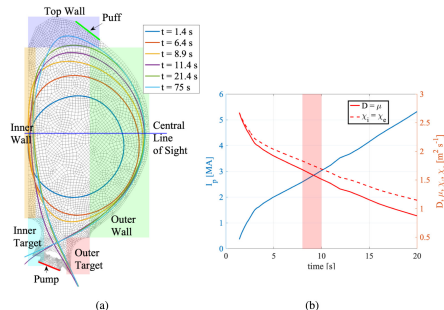


Figure: M. Scotto d'Abusco *et al.*, First integrated core-edge fluid simulation of ITER's Limiter-Divertor transition with SolEdge-HDG, Nuclear Materials and Energy 2024

SolEdge-HDG - Time-varying magnetic configurations

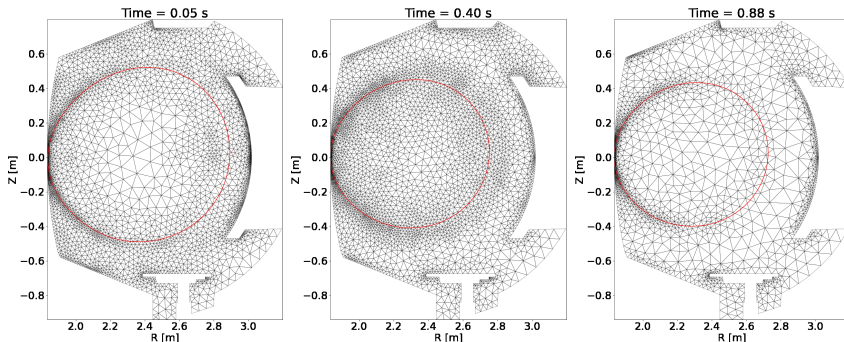
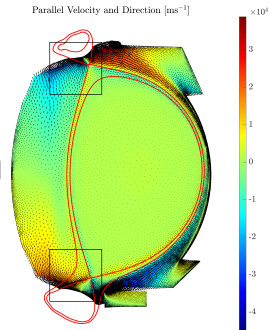


Figure: Modelling of limiter phase of start-up in WEST (I. Kudashev *et al.*, Nuclear Fusion, Volume 66, Number 7)

- computation of plasma transport "equilibria" throughout a plasma discharge,
- support for diagnostic interpretation,
- sensitivity analysis.

SolEdge-HDG takeaways

- Unstructured meshes allow accurate description of the wall
- High-order methods do reduce the computational cost of modelling
- Adaptive refinement is key to lowering computational cost and user time in transport modelling
- full-implicit advancement, though costly per iteration and in development, provides significant acceleration towards steady state.



Thank you for your attention !



Figure: Visible light imaging of the inside of tokamak WEST

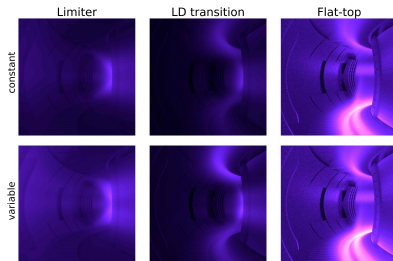


Figure: Visible light imaging reconstruction of the inside of tokamak WEST based on SolEdge-HDG computation (Ivan Kudashev)