BIEST: A High-Order Boundary Integral Equation Solver for Computing Taylor States in Stellarators

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Introduction

Computing Taylor states or force-free fields is an essential component in computing ideal magnetohydrodynamic (MHD) equilibrium. We present BIEST (Boundary Integral Equation Solver for Taylor states), a new numerical solver for the fast and accurate computation of Taylor states in toroidal geometries. Our boundary integral equation formulation has several advantages,

- **unknowns only on the boundary** leading to significant savings in work
- **well-conditioned system** due to second-kind integral equation formulation
- **high-order accurate** due to spectral discretization and special quadratures

Taylor States in Toroidal Geometries

In a bounded domain Ω, for a given value of the Beltrami parameter λ, the magnetic field $\mathbf{B}$ for Taylor states is described by the equations,

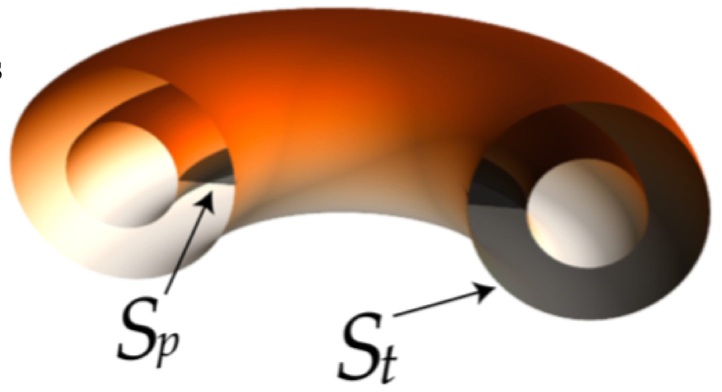
$$\nabla \times \mathbf{B} = \lambda \mathbf{B} \quad \text{in } \Omega$$

$$\mathbf{B} \cdot \mathbf{n} = 0 \quad \text{on } \Gamma.$$

In addition, the toroidal and poloidal flux conditions must be specified,

$$\int_{S_t} \mathbf{B} \cdot da = \phi^{tor}$$

$$\int_{S_p} \mathbf{B} \cdot da = \phi^{pol}.$$



Generalized Debye Formulation

We represent magnetic field $\mathbf{B}$ using the generalized Debye source representation of [1],

$$\mathbf{B} = i\lambda \mathbf{Q} - \nabla v + i\nabla \times \mathbf{Q}$$

where, $\mathbf{Q}$ and v are vector and scalar potentials given by the surface convolutions,

$$\mathbf{Q}(\mathbf{x}) = \int_\Gamma \frac{e^{ik|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|}\, \mathbf{m}(\mathbf{x}')\, da', \qquad v(\mathbf{x}) = \int_\Gamma \frac{e^{ik|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|}\, \sigma(\mathbf{x}')\, da'.$$

For the Taylor state condition ($\nabla\times\mathbf{B} = \lambda\mathbf{B}$) to hold, we require the consistency conditions,

$$\nabla_\Gamma \cdot \mathbf{m} = i\lambda\sigma, \qquad \mathbf{n} \times \mathbf{m} = i\, \mathbf{m}.$$

Then, from the consistency conditions,

$$\mathbf{m} = i\lambda \left(\nabla_\Gamma \Delta_\Gamma^{-1}\sigma - i\, \mathbf{n} \times \nabla_\Gamma \Delta_\Gamma^{-1}\sigma \right) + \alpha\, \mathbf{m}_H$$

where,

∇_Γ : surface gradient operator

Δ_Γ^{-1} : inverse of surface Laplacian (restricted to mean-zero functions)

$\mathbf{m}_H$ are tangential harmonic vector field such that $\nabla_\Gamma \cdot \mathbf{m}_H = 0$, $\mathbf{n} \times \mathbf{m}_H = i\, \mathbf{m}_H$.

Boundary Integral Equation Formulation

Applying the boundary conditions ($\mathbf{B} \cdot \mathbf{n} = 0$ on Γ), results in a **second-kind** integral equation,

$$\sigma/2 + i\lambda \mathbf{n} \cdot \mathcal{S}_\lambda[\mathbf{m}] - \mathbf{n} \cdot \nabla \mathcal{S}_\lambda[\sigma] + i\mathbf{n} \cdot \nabla \times \mathcal{S}_\lambda[\mathbf{m}] = 0.$$

Flux conditions: computed from circulation on the boundary of a cross-section,

$$\int_S \mathbf{B} \cdot d\mathbf{a} = \frac{1}{\lambda} \oint_{\partial S} \mathbf{B} \cdot d\mathbf{l} \qquad (\nabla \times \mathbf{B} = \lambda \mathbf{B},\ \text{Stokes' theorem}).$$

Discretize and solve for the unknowns σ and $\{\alpha_1, \alpha_2\}$ using GMRES,

$$\begin{bmatrix} \mathbf{A} & \mathbf{u_1} & \mathbf{u_2} \\ \mathbf{v_1^T} & c_{11} & c_{12} \\ \mathbf{v_2^T} & c_{21} & c_{22} \end{bmatrix} \begin{bmatrix} \sigma \\ \alpha_1 \\ \alpha_2 \end{bmatrix} = \begin{bmatrix} 0 \\ \phi^{tor} \\ \phi^{pol} \end{bmatrix}.$$

Boundary Integral Equation Solver

A boundary integral solver of axisymmetric toroidal geometries was presented in [2]. We extend this to a fully three-dimensional solver. This required efficient discretization of the surface, a fast Laplace-Beltrami solver (to apply Δ_Γ^{-1}) and high-order singular quadratures (to apply $\mathcal{S}_\lambda$) in 3D.

Surface Discretization

Each toroidal surface is parameterized by toroidal angle (θ) and the poloidal angle (ϕ). We use Fourier discretization for the surface position and density functions.

$$f(\theta, \phi) \approx \sum_{n=0}^{N_\theta-1} \sum_{m=0}^{N_\phi-1} \widehat{f}_{nm} e^{i(n\theta + m\phi)} \qquad \text{where,} \quad \widehat{f}_{nm} = \frac{1}{2\pi N_\theta N_\phi} \sum_{i=0}^{N_\theta-1} \sum_{j=0}^{N_\phi-1} f_{ij} e^{i(n\theta_i + m\phi_j)}$$

Laplace Beltrami Solver

We use spectral differentiation in Fourier space to evaluate derivatives,

$$\mathbf{f}_\theta = \mathbf{D}_\theta \mathbf{f} = \mathcal{F}^{-1} \widehat{\mathbf{D}_\theta} \mathcal{F}\mathbf{f}, \qquad \mathbf{f}_\phi = \mathbf{D}_\phi \mathbf{f} = \mathcal{F}^{-1} \widehat{\mathbf{D}_\phi} \mathcal{F}\mathbf{f}.$$

Operators $\mathcal{F}$ and $\mathcal{F}^{-1}$ are accelerated using the **Fast Fourier Transform (FFT)**.
The discrete Laplace Beltrami operator (Δ_{Γ_h}) is then defined as,

$$\nabla_{\Gamma_h} \mathbf{u} = \left[\mathbf{x}_\theta \mathbf{x}_\phi\right] \mathbf{G}^{-1} \begin{bmatrix} \mathbf{D}_\theta \\ \mathbf{D}_\phi \end{bmatrix} \mathbf{u}, \qquad \nabla_{\Gamma_h} \cdot \mathbf{v} = \frac{1}{\sqrt{|\mathbf{G}|}} \left[\mathbf{D}_\theta \mathbf{D}_\phi\right] \sqrt{|\mathbf{G}|}\, \mathbf{v}, \qquad \Delta_{\Gamma_h} \mathbf{u} = \nabla_{\Gamma_h} \cdot \nabla_{\Gamma_h} \mathbf{u}$$

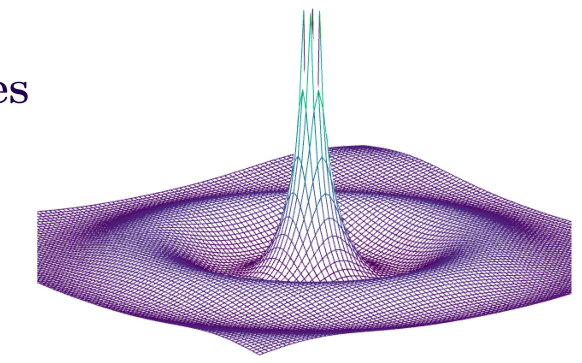
where, $\mathbf{G}$ is the metric tensor.

- **Spectral Preconditioner:** exact inverse $\Delta_{\Gamma_h}^{-1}$ for flat surface (from [3]).
- **Solve:** $(\Delta_{\Gamma_h} + \mathbf{1}\mathbf{w}^\mathbf{T})\mathbf{u} = \mathbf{f}$ using BiCG-stab or GMRES

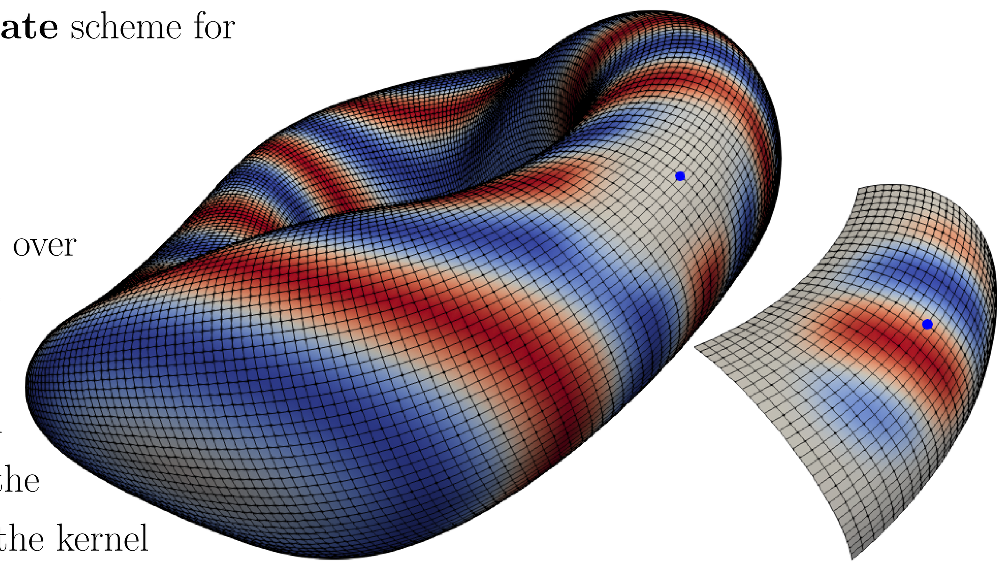
High-Order Singular Quadratures on Surfaces

Evaluating layer potential due to singular kernel functions $\mathcal{S}(\mathbf{r})$ requires special quadratures.

$$\mathcal{S}[f](\mathbf{x}) = \int_\Gamma \mathcal{S}(\mathbf{x} - \mathbf{x}') f(\mathbf{x}') da', \qquad \mathcal{S}(\mathbf{r}) = \frac{e^{ik|\mathbf{r}|}}{4\pi|\mathbf{r}|} =$$



We present a **fast**, **high-order accurate** scheme for computing such integrals.



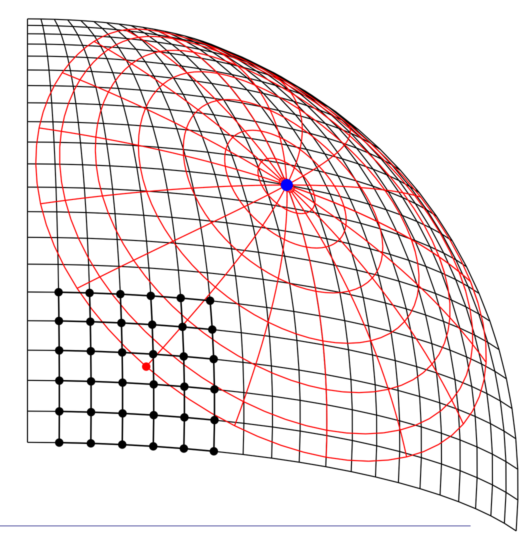
Partition of unity function

Split the integral into a smooth integral over the entire surface Γ and a local singular integral using a smooth partition of unity function $\eta_\mathbf{x}$. The singular integral is computed in polar coordinates since the Jacobian of the transformation cancels the kernel singularity.

$$\mathcal{S}[f](\mathbf{x}) = \underbrace{\int_\Gamma (1 - \eta_\mathbf{x}(\mathbf{x}'))\mathcal{S}(\mathbf{x} - \mathbf{x}')f(\mathbf{x}')da'}_{\text{(smooth - use trapezoidal rule can be accelerated using FMM)}} + \underbrace{\int_{B_\eta(\mathbf{x})} \eta_\mathbf{x}(\mathbf{x}')\mathcal{S}(\mathbf{x} - \mathbf{x}')f((x'))da'}_{\text{(singular - use polar coordinates)}}$$

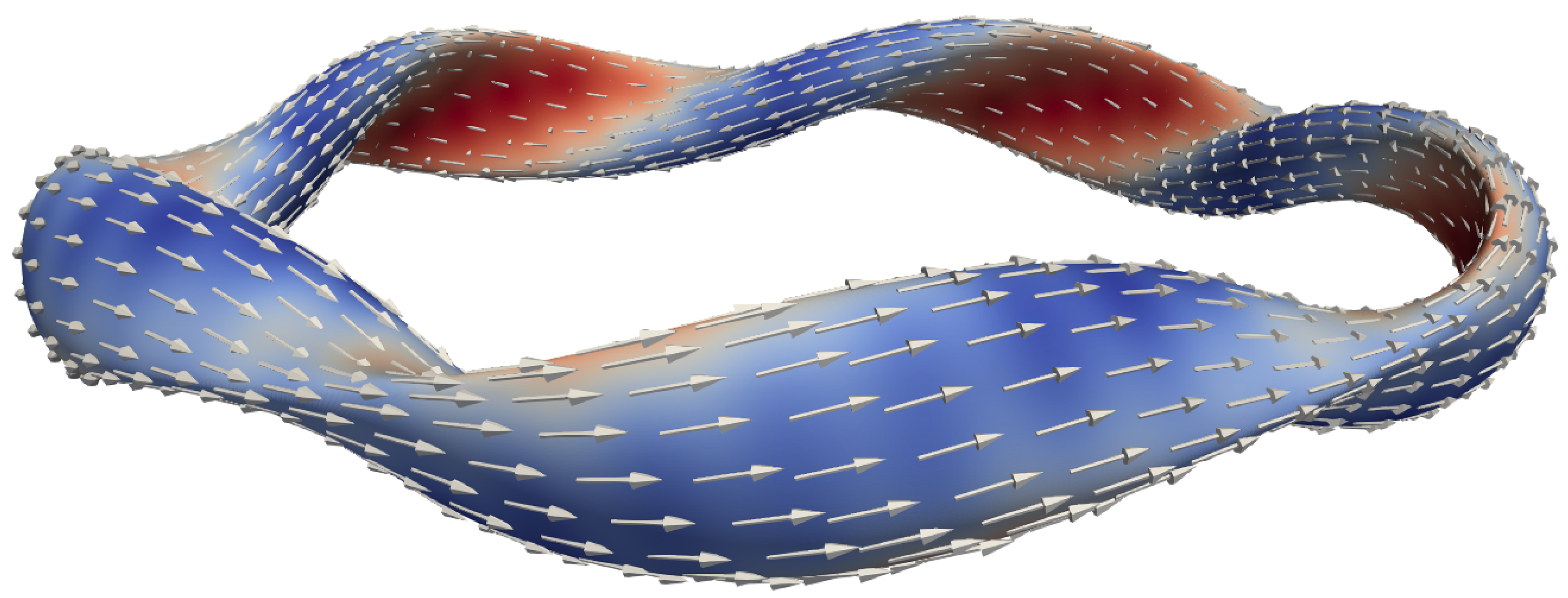
Polar quadrature scheme

- Interpolate from $M \times M$ grid to a polar grid using Lagrange interpolation.
- Use q-th order Gauss-Legendre quadrature in radial direction, $2q$-th order trapezoidal rule in angular direction.
- Pre-compute target-specific weights on the original $M \times M$ grid.



Numerical Results

We compare our boundary integral equation solver (BIEST) with the Galerkin code SPEC from [4] for the geometry defined by the outer surface of the Wendelstein 7-X stellarator. For both codes, we report the solve time and the L^∞-norm of the error compared to a reference solution. We show results for two cases: for $\lambda = 0$ (vacuum fields) and for $\lambda = 1$. All experiments were conducted on a 60-core Intel Ivy-Bridge machine.

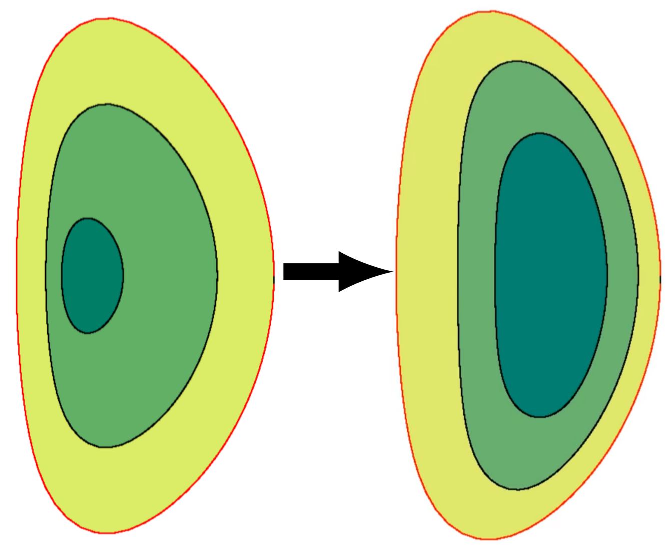


BIEST		$\lambda = 0$		$\lambda = 1$		SPEC	$\lambda = 0$		$\lambda = 1$	
N	ϵ_{GMRES}	$\lvert e\rvert_\infty$	T_{solve}	$\lvert e\rvert_\infty$	T_{solve}	$M_\phi \times M_\theta \times L_r$	$\lvert e\rvert_\infty$	T_{solve}	$\lvert e\rvert_\infty$	T_{solve}
3.9E+3	1E-01	8E-1	0.1	2E-1	1.0	11 × 11 × 5	3E-1	14	3E-1	13
8.8E+3	3E-02	2E-1	0.4	6E-2	4.4	13 × 13 × 5	6E-2	38	6E-2	38
2.5E+4	3E-03	3E-2	2.1	7E-3	29.8	15 × 15 × 5	8E-3	115	9E-3	118
3.5E+4	1E-03	7E-3	4.3	3E-3	61.6	21 × 21 × 5	2E-3	527	2E-3	541
9.8E+4	3E-05	2E-4	27.3	1E-4	492.1	-	-	-	-	-
1.9E+5	1E-06	9E-6	98.1	9E-6	1991.0	-	-	-	-	-
7.7E+5	1E-09	5E-9	1309.1	2E-9	40646.2	-	-	-	-	-

- Our boundary integral scheme converges to about 9-digits while the Galerkin approach of SPEC stops converging with mesh refinement beyond 3-digit accuracy due to ill-conditioned of the system.
- For the same solution accuracy, BIEST is nearly 100× faster for the vacuum field case and about 8× faster for $\lambda > 0$. Unlike SPEC, we currently do not take advantage of the 5-fold symmetry of the W7X stellarator and this could give us another 5× speedup.

Future Work

- **Adaptive meshes and surfaces with edges:** to resolve sharp features close to the divertor.
- **Near-singular quadratures:** to efficiently compute layer-potentials when surfaces get very close.
- **Estimate Hessian:** to accelerate the stepped-pressure equilibrium computation.



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