Accurately calculating equilibrium quantities with any Grad-Shafranov solver

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Motivation

A common circumstance in plasma physics is:

- Potential ψ solves an elliptic PDE
- Physical quantities that are needed for wave, stability, transport calculations are $\nabla\psi$, $D^2\psi$, etc...

Finite element/finite difference based solvers lose an order of accuracy for every derivative taken.

Can we find a way to obtain derivatives to the same order accuracy as the solution itself, **while using these same finite element/finite difference solvers**?

We show here that the answer is **YES!**

We demonstrate how this works for the Grad-Shafranov equation

GRAD-SHAFRANOV EQUATION

- 2-D axisymmetric equilibria are determined by solving the *Grad-Shafranov equation*,

$$x\frac{\partial}{\partial x}\left(\frac{1}{x}\frac{\partial\psi}{\partial x}\right)+\frac{\partial^2\psi}{\partial y^2}=-\mu_0 x^2\frac{dp}{d\psi}-\frac{1}{2}\frac{dI^2}{d\psi} \tag{1}$$

- $\nabla\psi$ determines magnetic field, $D^2\psi$ determines *stability* $\implies$ Accurate derivative information is critical.
- Standard FEM codes [1,2]: fixed pt. iteration, bicubic-Hermite basis, isoparametric coordinates $\implies$ 4^{th} order in ψ $\implies$ only 2^{nd} order in $D^2\psi$.

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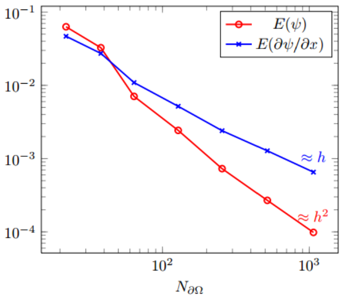
[1]CHEASE: H. Lütjens, A. Bondeson, A. Roy, *Computer Physics Communications* **69**, 287 (1992)

[2]FINESSE: A.J.C. Beliën, M.A. Botchev, J.P. Goedbloed, B. van der Holst, and R. Keppens, *Journal of Computational Physics* **182**, 91 (2002)

Loss of accuracy for equilibrium quantity



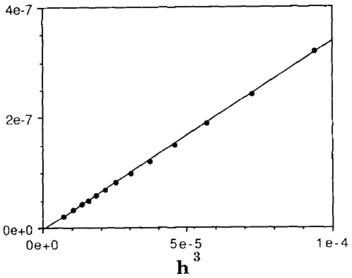


Figure on the left: loss of accuracy from ψ to $\partial\psi/\partial x$ for the 2nd order accurate FEM solver FreeFem++[3]

Figure on the right: loss of accuracy for the location of the magnetic axis for the 4th order accurate FEM solver CHEASE[1]

[3]E. Deriaz *et. al.*, CEMRACS'10 research achievements: numerical modeling of fusion, 76-94, ESAIM Proc., 32, EDP Sci., Les Ulis, 2011.

Main ideas

1. Change of variable $u \equiv \psi/\sqrt{x}$, so u satisfies a nonlinear Poisson equation:

$$\Delta u = \frac{3}{4}\frac{u}{x^2} - \mu_0 x \frac{dp}{du} - \frac{1}{2x}\frac{dI^2}{du} \equiv F(x,y,u) \tag{2}$$

2. Instead of differentiating the solution numerically, differentiate the PDE itself. For example, if u solves (2), then u_x solves

$$\Delta u_x - F_u(x,y,u)u_x = F_x(x,y,u) \tag{3}$$

- Use FEM to solve (2) for u.
- Use *same* FEM solver - along w/ now known u - to solve (3) for u_x to *same order*.
- Missing piece: Dirichlet boundary data for u_x.

Boundary Data & Dirichlet to Neumann map

Tangential derivative u_t can be computed by spectral differentiation without losing an order

Problem boils down to computing normal derivative u_n accurately. This is how it works

- Set $u = u^h + u^p$, with

$$u^p = \int_\Omega G(\mathbf{x}, \mathbf{x}')F(\mathbf{x}', u(\mathbf{x}'))\, d\mathbf{x}' \tag{4}$$

  and u^h harmonic: $\Delta u^h = 0$.
- Introduce new variable U^h such that $\nabla^\perp U^h = \nabla u^h$ (Harmonic conjugate of u^h)
- U^h satisfies $\Delta U^h = 0$ and $U^h_t = u^h_n$.

Boundary Data & Dirichlet to Neumann map

- Differentiate (4) analytically and evaluate integral $\rightarrow u_n^p$.
- By Green's second identity, for any $\mathbf{x}$ on the boundary $\partial\Omega$, U^h solves the following second-kind integral

$$\frac{1}{2}U^h(\mathbf{x}) + \int_{\partial\Omega} G_n U^h(\mathbf{x}')dl' = \int_{\partial\Omega} G U_n^h(\mathbf{x}')dl' = -\int_{\partial\Omega} G u_t^p(\mathbf{x}')dl' \tag{5}$$

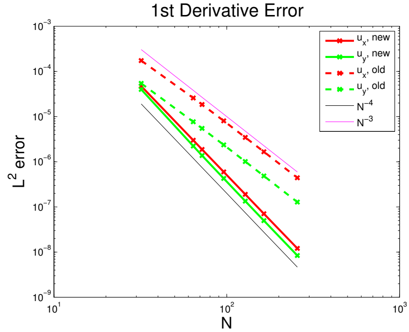
- Once we know U^h, we can take spectral derivative to obtain $U_t^h = u_n^h$ accurately on the boundary.

Execution requires accurate evaluation of singular integrals - e.g. (4). We use FMM accelerated Quadrature by Expansion (QBX) [4].

Computational complexity of entire process **comparable to one FEM solve.**

[4] A.Klöckner, A.Barnett, L.Greengard, M.O'Neil, *Journal of Computational Physics* **252**, 332 (2013)

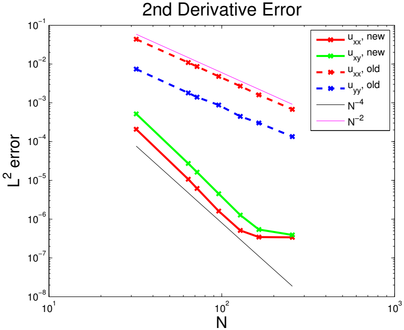
Numerical Results



Errors in derivatives of the solution of (2) using direct differentiation of the FEM solution (old) and the method presented here (new). N is the number of grid points in each direction.

∇u errors, demonstrating the expected 3$^{\text{rd}}$ order convergence for the naive approach, and 4$^{\text{th}}$ order for our method.

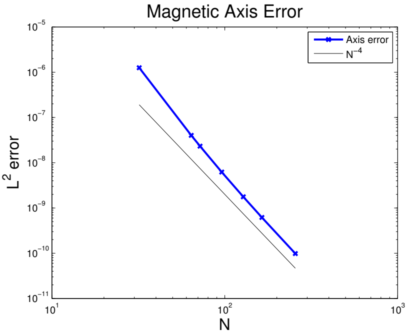
NUMERICAL RESULTS



Errors in derivatives of the solution of (2) using direct differentiation of the FEM solution (old) and the method presented here (new). N is the number of grid points in each direction.

D^2u errors, demonstrating expected two order of accuracy improvement. The leveling-off is due to round-off error, the effect of which is amplified by taking repeated spectral derivatives.

Application - Magnetic Axis



Computation of the location of the magnetic axis requires accurate values of $\nabla\psi$.
The above plot demonstrates 4$^{\text{th}}$ order convergence in this quantity, in contrast to the 3$^{\text{rd}}$ order accuracy observed with CHEASE[1] using the same FEM solver.

Summary

- We have demonstrated a technique for computing derivatives of a FEM solution whose **loss in accuracy of only a constant factor, rather than an order of accuracy in N**.
- The new method increases the overall complexity of the computation by an amount comparable to a single additional FEM solver per derivative computed.
- **The new method achieves an accuracy at $N = 128$ that would require $N \approx 5000$ to reach via direct differentiation**, while adding only small additional computational complexity to the problem.
- The method is iterable to an arbitrary number of derivatives, and is independent of the order of the FEM solver. It can thus be used as a **plug-in to existing FEM Grad-Shafranov or Poisson solvers**.