Numerical Demands of Systems with High-Order Derivatives
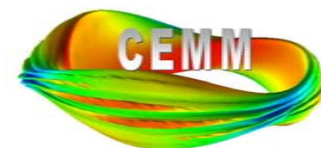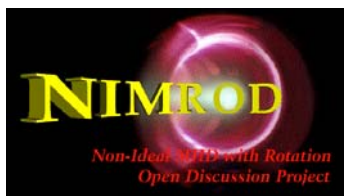
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Closures Workshop

Oak Ridge National Laboratory

March 22-24, 2006

Outline

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    - Theoretical development
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- Spatial representation
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- Discussion

Introduction

Analytical work for extended-MHD can be summarized for the non-specialist as:

• Macroscopic dynamics involve changes in the magnetic field (and topology).

• Electromagnetics only cares about sums of the lowest-order velocity moments of the particle distributions.

• The most concise description of macroscopic dynamics is expected to be from moment-based evolution equations. (?)

    • Closure relations are needed to model the influence of distribution-function details on low-order moment evolution.

    • Large effective mean-free-path and gyro-orbit effects preclude simple relations; we will likely see research continuing for many years.

High-Order Derivatives

Even relatively simple models can lead to high-order derivatives:

• For collisional plasmas, the electron parallel stress, for example, is proportional to

$$\hat{\mathbf{b}} \cdot \underline{\underline{\mathbf{W}}}_e \cdot \hat{\mathbf{b}} \left(\hat{\mathbf{b}}\hat{\mathbf{b}} - \frac{1}{3}\mathbf{I} \right), \quad \underline{\underline{\mathbf{W}}}_e \equiv \nabla \mathbf{V}_e + \left(\nabla \mathbf{V}_e \right)^T - \frac{2}{3}\mathbf{I}(\nabla \cdot \mathbf{V}_e)$$

• Using $\mathbf{V}_{\text{COM}}$ and $\mathbf{J}$ instead of $\mathbf{V}_i$ and $\mathbf{V}_e$ is advantageous for low frequency (no displacement current), but $\mathbf{W}_e$ then contains terms

$$\nabla \left(\mathbf{V} - \frac{1}{ne}\mathbf{J} \right) = \nabla \left(\mathbf{V} - \frac{1}{\mu_0 ne} \nabla \times \mathbf{B} \right)$$

• With $\mathbf{E}$ proportional to the divergence of electron stress, the combined Faraday's/Ohm's evolution equation for $\mathbf{B}$ has four spatial derivatives on $\mathbf{B}$.

• Even if we're not interested in collisional behavior, related collisional operators may be needed for semi-implicit advances or 'physics-based' preconditioning.

Computation: ideal situation

In a perfect computational world, the hard work would be done once we know the system of equations:

• We would be able to program any nonlinear PDE or integro-differential system easily.

• The code would run efficiently on laptops, massively parallel architectures, and whatever performance machines will be like in the next 5-10 years.

• We would achieve qualitatively correct results at low spatial and temporal resolution.

• We would achieve quantitatively correct results at high resolution.

• Convergence from low resolution to high resolution would be rapid.

Computation: reality

In the real computational world, the hard work is not over once we know the system of equations:

• Even the simplest description of macroscopic dynamics, MHD, presents challenges for numerical computation.

- • Stiffness
- • Anisotropy
- • Nonlinearity
- • Geometry (device and equilibrium)
- • Divergence constraint

• Increasing the complexity of the model compounds the first three and makes verification increasingly difficult.

• Present-day temporal algorithms rely on specially tailored advances or preconditioners.

• The spatial mesh cannot be perfectly aligned with **B**.

Spatial Representation

Element-based methods are favored (M3D & NIMROD and don't forget eigenvalue codes ER/G-ATO, PEST, etc.):

• Modeling complicated geometries is relatively straightforward.

• Self-adjoint differential operators lead to symmetric or Hermitian matrices, by construction, in the discrete representation.

  • Eigenvalues of the respective operators remain real.

  • Maintaining this property with finite differences can be quite challenging.

• Boundary conditions are either built into the solution space or addressed by surface integrals.

  • There are no ghost points or 1-sided differences.

• High-order finite volume methods are related.

• There are spectral versions of the method.

Element Basis Functions

• Local representations must include the lowest-order polynomials to guarantee convergence (connection to Taylor expansion).

• Polynomial basis functions (uniform Lagrange, Gauss-Lobatto-Legendre, modal) may have degree>1:

- **Control magnetic divergence error**
- **Put curvature in mappings**
- **Achieve high-order convergence without uniform meshing**
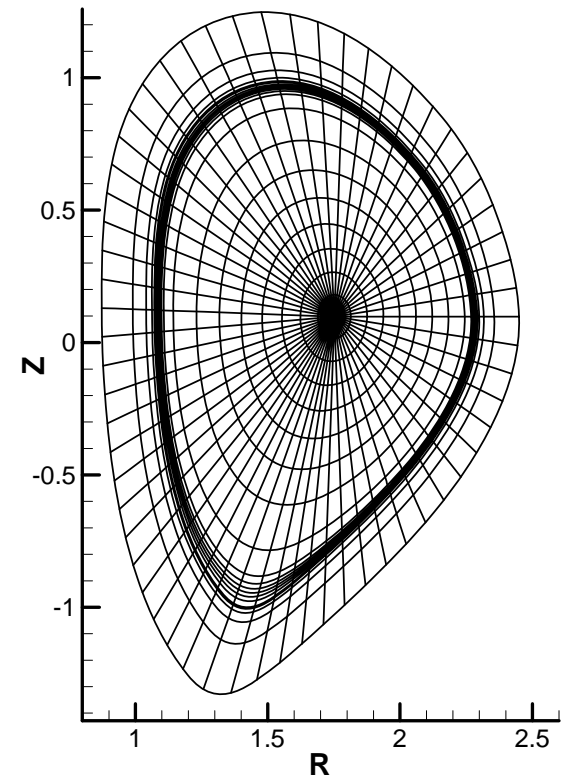
Packed mesh for DIII-D ELM study
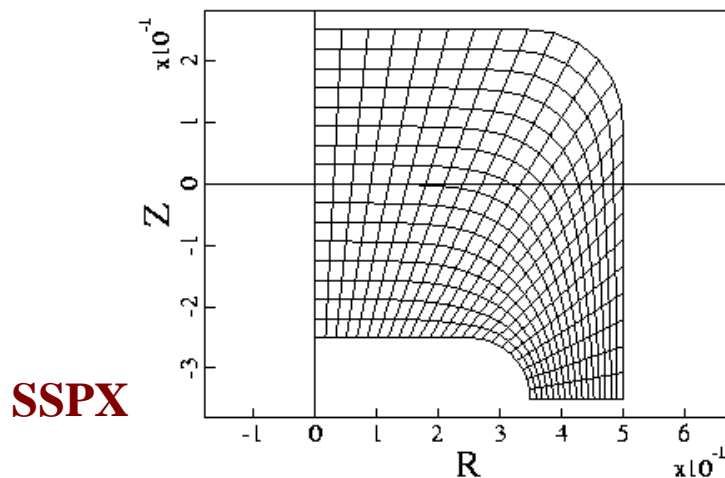
SSPX
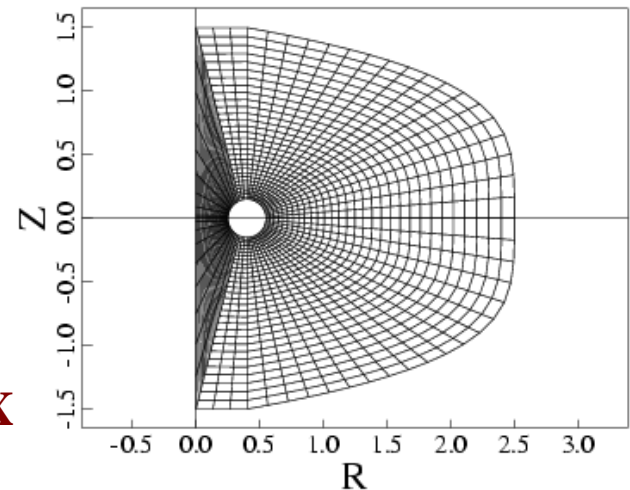
LDX

High-Order Bases: constraint relations

'Error diffusion' is added to Faraday's law:

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} + \kappa_{divb} \nabla \nabla \cdot \mathbf{B}$$
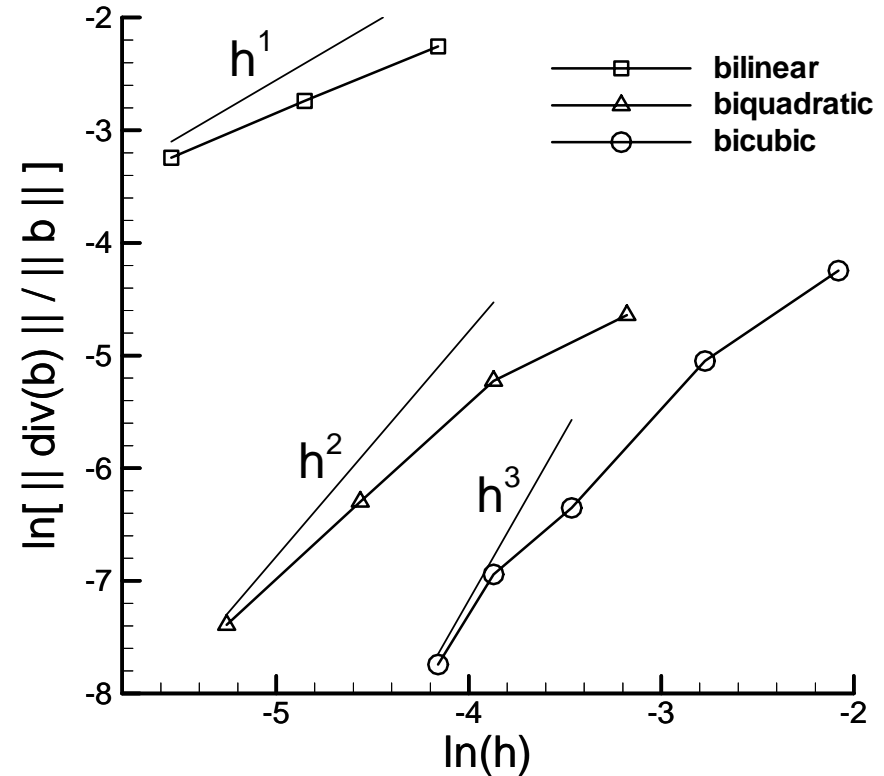
$$\int d\mathbf{x} \left\{ \mathbf{c}* \cdot \Delta \mathbf{b} + g \Delta t \, \kappa_{divb} (\nabla \cdot \mathbf{c}*)(\nabla \cdot \Delta \mathbf{b}) \right\}$$

$$= \Delta t \int d\mathbf{x} \left\{ \kappa_{divb} (\nabla \cdot \mathbf{c}*)(\nabla \cdot \mathbf{b}) - (\nabla \times \mathbf{c}*) \cdot \mathbf{E} \right\}$$

$$- \Delta t \oint d\mathbf{s} \times \mathbf{E} \cdot \mathbf{c}*$$

for all vector test functions **c***.

The ratio of DOF/constraints is 3 in the limit of large polynomial degree.
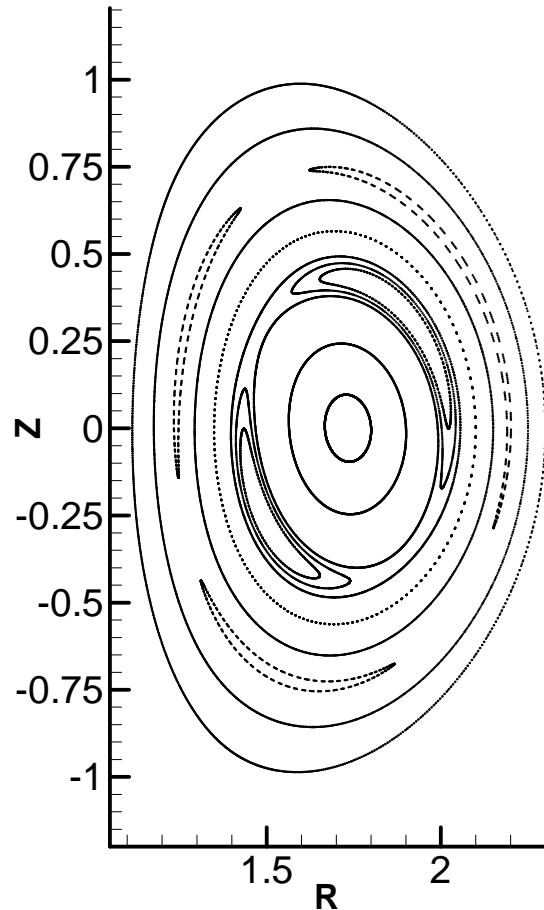

Magnetic divergence in a tearing-mode calculation.

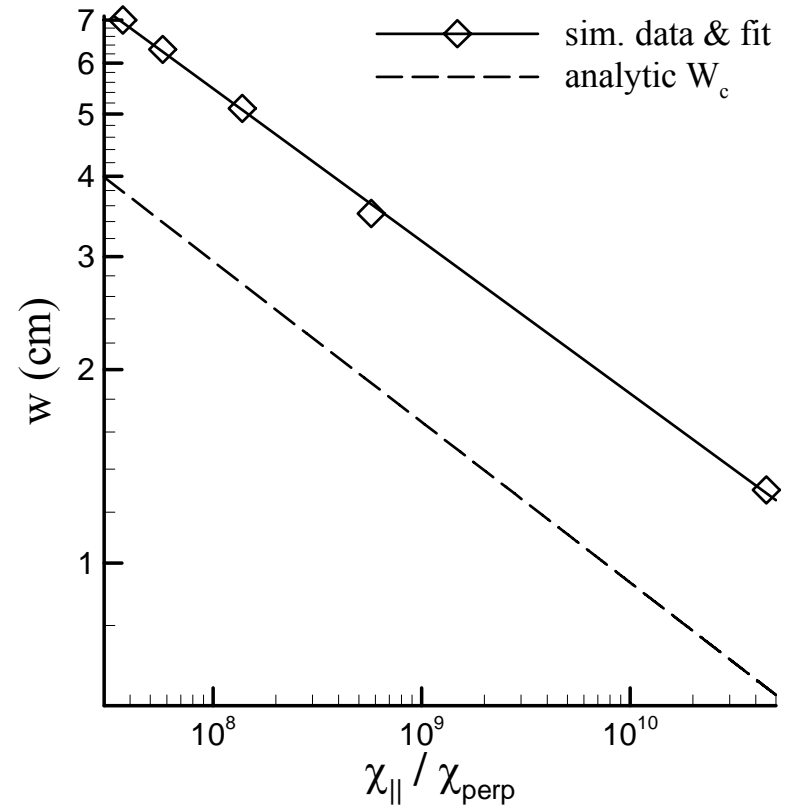Scalings show convergence rates expected for first derivatives.

High-Order Bases: resolution of extreme anisotropy

This test solves $\nabla \cdot \left[\left(\chi_{\parallel} - \chi_{\perp} \right) \hat{\mathbf{b}}\hat{\mathbf{b}} + \chi_{\perp} \mathbf{I} \right] \cdot \nabla T = 0$ with an island.

[JCP **195**, 355, 2004]

Critical island width vs. $\chi_{\parallel}/\chi_{perp}$

With anisotropy, heat transport across magnetic islands is a competition between parallel and perpendicular processes.

Numerical results are from bicubic polynomials. W_c shows where diffusion time-scales match [Fitzpatrick, PoP **2**, 825 (1995)].

Finite Element Solution Properties

Solution spaces are central to the finite element method, but the differential operators in the system influence which spaces are suitable.

• Analytically, $\hat{\mathbf{b}} \cdot \nabla$ in the MHD force perturbation, thermal conduction, and other operators leads to distinct modes.

• Numerically, we apply these operators to finite-dimensional spaces that do not have the same 'flexibility.'

    • Though local, polynomial bases do a poor job of representing delta functions at $\hat{\mathbf{b}} \cdot \nabla$ resonances (singular effects).

    • Standard polynomial-space *solutions* of weak-form equations do not separate precisely into longitudinal and solenoidal parts.

• Special low-order spaces and approximations were developed for ideal-MHD eigenvalue computations to avoid artificial coupling of shear & compression.

Requirements for the Method

Standard methods and analyses rest on *conforming* approximations.

(conforming meaning that the finite-dimensional spaces belong to the same space as that of the analytical Galerkin problem)

- If the original PDE system $D(u) = f$ has derivatives of order $2m$ appearing explicitly, the weak form requires square-integrable derivatives of order m.

  - Expansion of the space relies on completeness
  - Necessary for identifying good solutions (weak form of the operator creates a norm, at least in symmetric problems)
  - Examples:
    - m=1 for visco-resistive MHD with primitive variables
    - m=2 for same with a potential rep.
    - m=2 with electron viscosity and primitive variables.

  - Implies C^{m-1} continuity is required.

- A *regular* (not uniform) discretization is also required.

Present Modeling

Present numerical models (speaking for NIMROD, at least) are not perfect.

• To allow for viscosity and diffusive thermal conduction, NIMROD presently uses C^0 for all fields.

• We have found that time-dependent problems are not as exacting on the spaces as the ideal-MHD eigenvalue computations, where marginal conditions are scanned.

• However, if resonances are inadequately resolved, the system acts as if it were ideal, where the C^0 space leads to unphysical couplings.

Future Modeling

We must reconsider the solution space when adding new closures.

Adding closures with high derivatives certainly requires change:

• Solution spaces either needs greater continuity (not trivial) …

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} \sim -\nabla \times \frac{1}{ne} \nabla \cdot \mu_e \nabla \left(\mathbf{V} - \frac{1}{\mu_0 ne} \nabla \times \mathbf{B} \right)$$

FE & time-discrete with C^1 continuity requirements:

$$\int dVol \left(\mathbf{C} \cdot \Delta \mathbf{B} - \frac{\Delta t \mu_e}{\mu_0} \nabla \left(\frac{1}{ne} \nabla \times \mathbf{C} \right)^T : \nabla \left(\frac{1}{ne} \nabla \times \Delta \mathbf{B} \right) \right)$$

$$= \int dVol \frac{\Delta t \mu_e}{\mu_0} \nabla \left(\frac{1}{ne} \nabla \times \mathbf{C} \right)^T : \nabla \left(\mathbf{V} - \frac{1}{\mu_0 ne} \nabla \times \mathbf{B}^{old} \right)$$

for all vector functions $\mathbf{C}$ in the same polynomial space as $\mathbf{B}$.

… or …

Future Modeling: continued

• We have to add to the number of fields being solved simultaneously, the rate of strain tensor in this example:

$$\int dVol \left(\mathbf{C} \cdot \Delta \mathbf{B} + \frac{\Delta t \mu_e}{ne} \nabla \times \mathbf{C} \cdot \left(\nabla \cdot \Delta \underline{\underline{\mathbf{W}}}_e \right) \right) = -\int dVol \frac{\Delta t \mu_e}{ne} \nabla \times \mathbf{C} \cdot \left(\nabla \cdot \underline{\underline{\mathbf{W}}}_e{}^{old} \right)$$

$$\int dVol \left(\underline{\underline{\mathbf{X}}} \cdot \Delta \underline{\underline{\mathbf{W}}}_e + \frac{1}{ne} \nabla \times \Delta \mathbf{B} \cdot \left(\nabla \cdot \underline{\underline{\mathbf{X}}} \right) \right) = 0$$

for all vector functions $\mathbf{C}$ in the same polynomial space as $\mathbf{B}$ and all $\underline{\underline{\mathbf{X}}}$ in the same space as $\underline{\underline{\mathbf{W}}}_e$.

This approach was used to test the Harned-Mikić semi-implicit Hall advance in NIMROD. Solving the larger system (with just a 3-vector auxiliary field) of equations was slower.

Summary & Discussion

• Finite elements can work well (geometry, anisotropy, etc.) on relatively simple systems of equations if we understand the properties of the operators and use this knowledge when constructing the finite-dimensional spaces.

• What will be the spectral properties of our new systems of equations?

• If we're not sure, or the answer is subject to frequent change, we may need to adapt a more robust representation. Possibilities include:

    • Spectral elements (very high order polynomials but presently low order continuity at macro-element interfaces)

    • Discontinuous Galerkin (high-order finite volume--keep inter-element surface integrals--mostly used for shock-capturing)

Can we close this gap?

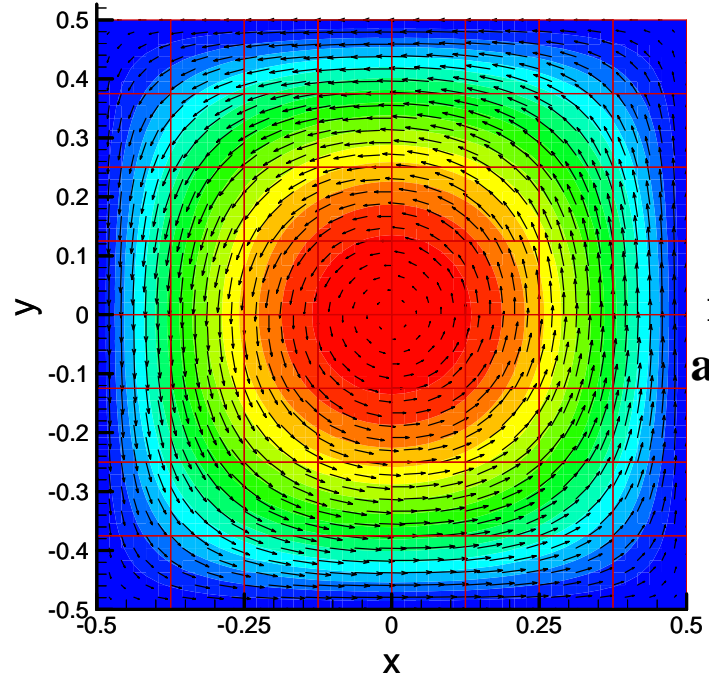Analytic theorist thinks, "Why are you solving an irrelevant system of equations?"

Computationalist thinks, "Why are you developing equations that will never be solved?"

**Resolution of extreme anisotropies (Lorentz force and diffusion)**

T and B fields from an 8×8 mesh of bicubic elements.

Simple 2D test:

• Homogeneous Dirichlet boundary conditions on T

• Heat and perpendicular current have sources. $\quad 2\pi^2 \cos(\pi x)\cos(\pi y)$

• Analytically, the solution is independent of $\chi_{\parallel}$,

$$T(x,y) = \chi_{\perp}^{-1}\cos(\pi x)\cos(\pi y)$$

• The resulting $T^{-1}(0,0)$ measures the effective $\chi_{\perp}$, including the numerical truncation error.

$\chi_{\parallel} = 10^9$
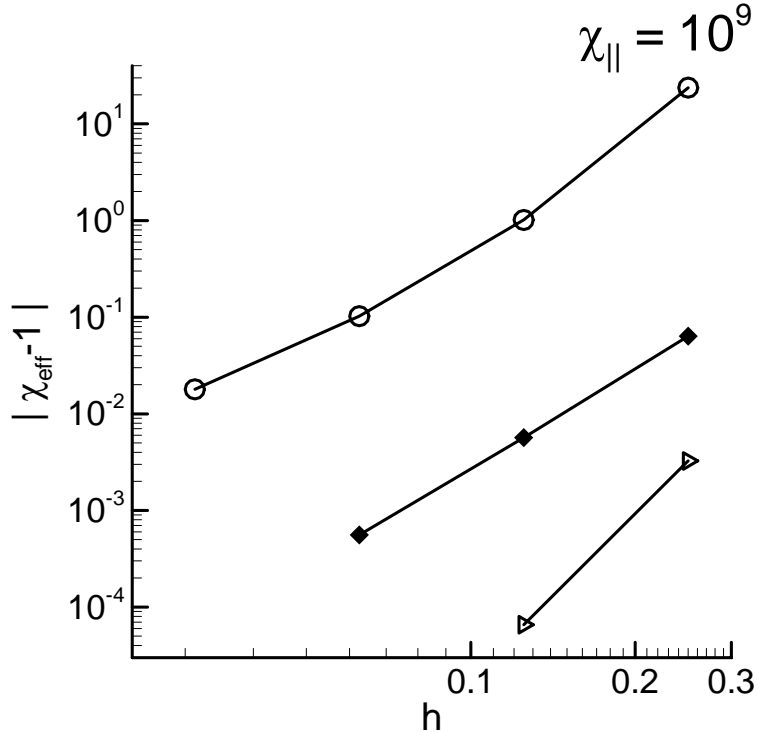
Diffusion error for bicubic, biquartic, and biquintic elements.