Generalized Vector Element Implementation and Optimization

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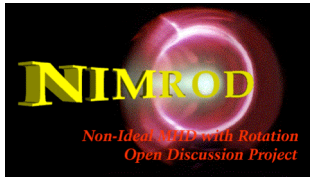
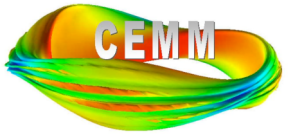
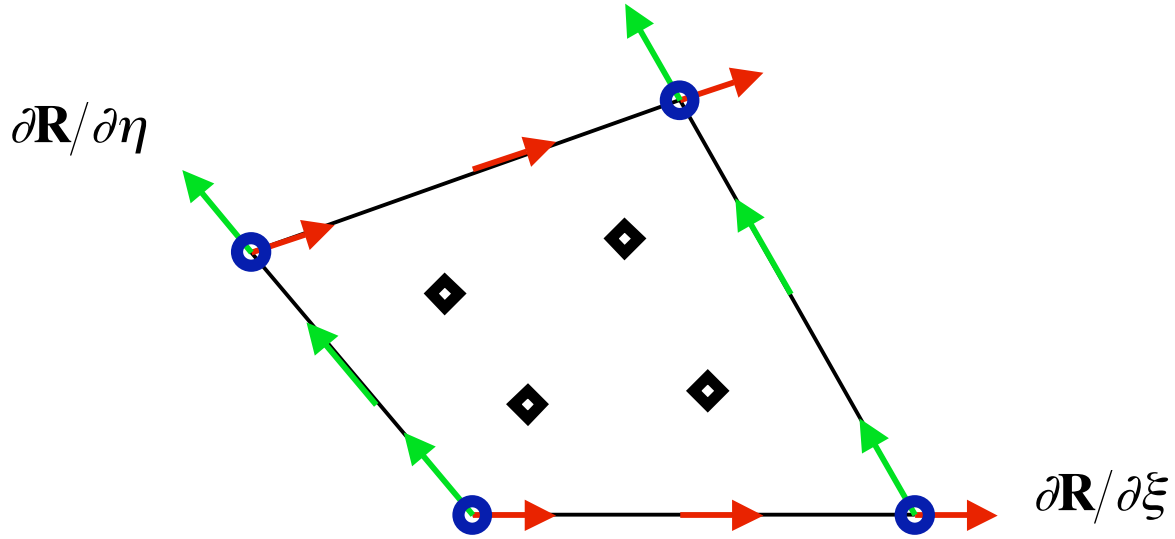




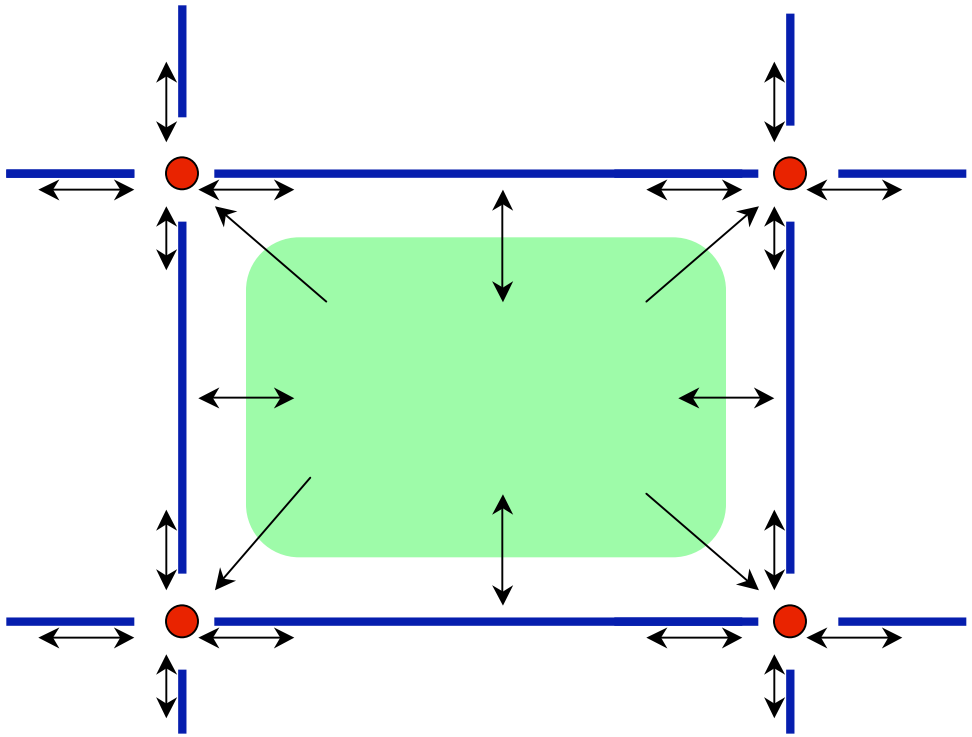
Vector-element implementation: Recall from CEMM (Monday) that we are studying a new representation.



- This sketch of a lowest-order biquadratic/bilinear element shows basis vectors at their node locations.
  - Circles are locations of continuous perpendicular components ($\partial\mathbf{R}/\partial\phi$).
  - Diamonds are nodes of scalars (discontinuous nodal).
- Maintaining structured data storage would be extremely complicated.
- Switching to element-based storage and element⇔global DOF mapping a la commercial FE codes is easier and adds flexibility.

The structure of NIMEIG parallels that of NIMROD, but some components differ substantially.

- There are modules or routines for quadrilateral elements, creating matrices, and evaluating integrands.
- Creating the element-to-global DOF table uses detailed mesh information.
  - 2D meshes are composed of vertices, edges, and elements.
  - Each vertex, edge, and element has a unique label.
  - Mesh_type module and mesh_init routine store and define connections.



… , but some components differ substantially, continued.

- The NIMEIG version of lagrange_quad contains separate modules for scalars and vectors that have $J\mathbf{A}\cdot\nabla u_i$ components.
- Because basis functions for scalars and different components of vectors are unique, basis information is in each derived-type definition for a data structure.
    - The data is self-describing.
    - Vector-calculus operators (gradient, divergence, curl) are part of the respective field module.
        - Divergence and curl are part of the vector-field module; gradient is part of the scalar-field module.
        - This makes the coding more object-oriented.
        - Integrand routines invoke differential operations for the respective type of field (scalar, $J\mathbf{A}\cdot\nabla u_i$-vector).
- Geometry information for each element is saved by element and is built upon the scalar data type.
    - This is analogous to Alan Glasser's old tgeom type.

… , but some components differ substantially, continued.

- With different fields having different nodes, NIMROD's existing boundary module for essential conditions won't work.
  - Essential conditions are identified on edges and vertices in the mesh.
  - They are transferred to element information and used in defining the element-to-global DOF table. Element DOFs that are eliminated by essential conditions are left out of the table.

(Repeat of CEMM:) Next steps with NIMEIG include …

- Checking for unphysical 0-frequency modes and spectral pollution in uniform-**B** conditions
    - Post-processing to separate different *k*-values is needed
- Incorporating the complete ideal-MHD system for nontrivial equilibria and the parallel-vorticity penalty equation
- Completing the element-to-global matrix relations for changes in basis vectors between adjacent elements
- Coupling to SCALAPACK or other parallel eigenvalue solvers for larger systems
- Technology transfer to NIMROD if or when results are sufficiently promising

Thoughts on transferring to NIMROD

- If the new representation passes NIMEIG testing, it can be tried in NIMROD.
- The approach would retain as much of the integrand and quad-point (field_comps--already element-based) computation as possible.
    - NIMEIG-type math operations on bases may simplify some aspects of integrand routines.
- With the element-to-global DOF map, matrices can go directly into condensed-column form, for example.
- With discontinuous scalars, their dissipation and advection need to be reformulated.

Optimization study: Ken Roche of PNL included NIMROD in his 2012 optimization effort for production science codes.

- It started the year as an OMB effort, but changes at OASCR altered the scale of the objectives.
- There are several NIMROD aspects.
  - Sherry Li is involved in migrating to new SLU_DIST and testing PDS_LIN.
  - Ken is investigating optimization of FE computation and static condensation.
  - Charlson has offered the particle module.
  - Cihan would like to improve HIT-SI simulation performance.
  - Jake is involved in OpenMP / MPI dual parallelization.