THE NIMROD CODE

The NIMROD Team

WHAT IS NIMROD?

- **AN ACRONYM:**

Non-Ideal MHD with Rotation: Open Discussion

- **A CODE:**

To simulate non-ideal (resistive, neo-classical), linear and non-linear, time-dependent, 3-D fluid effects in realistic geometry

- **A PROCESS:**

Employ Concurrent Engineering/Quality Function Deployment (QFD) team techniques to reduce code design and development time within the Fusion Program

- **A TEAM:**

Self-directed, interdisciplinary, multi-institutional, geographically diverse

THE CUSTOMER IS A CRUCIAL MEMBER OF THE TEAM!

THE NIMROD TEAM

Dan Barnes	**LANL**
Curt Bolton	**DOE/OFE**
Ming Chu	**GA**
Jim Crotinger	**LLNL**
Tom Gianakon	**U. Wisc.**
Alan Glasser	**LANL**
Harsh Karandakar	**SAIC**
Alice Koniges	**LLNL**
Rick Nebel	**LANL**
Mike Phillips	**Northrop Grumman**
Steve Plimpton	**SNL (ABQ)**
Olivier Sauter	**ITER**
Dalton Schnack	**SAIC**
Carl Sovinec	**LANL**
Alan Turnbull	**GA**

NIMROD TEAM FUNCTION

- WRITTEN GROUND RULES FOR TEAM INTERACTION

- SELF-DIRECTED

- SUB-GROUPS FOR PARTICULAR ISSUES
  - Gridding
  - Equations
  - Algorithms
  - Software Standards
  - CG and Parallel Computations

- ALL OPINIONS ARE VALUED

- DECISIONS ARE MADE BY CONSENSUS

  All team members must be able to "live with" any decision

- COMMUNICATION BETWEEN REMOTE SITES
  - E-mail
  - Bi-weekly tele-conference
  - Video-conference
  - Web site
  - Meetings

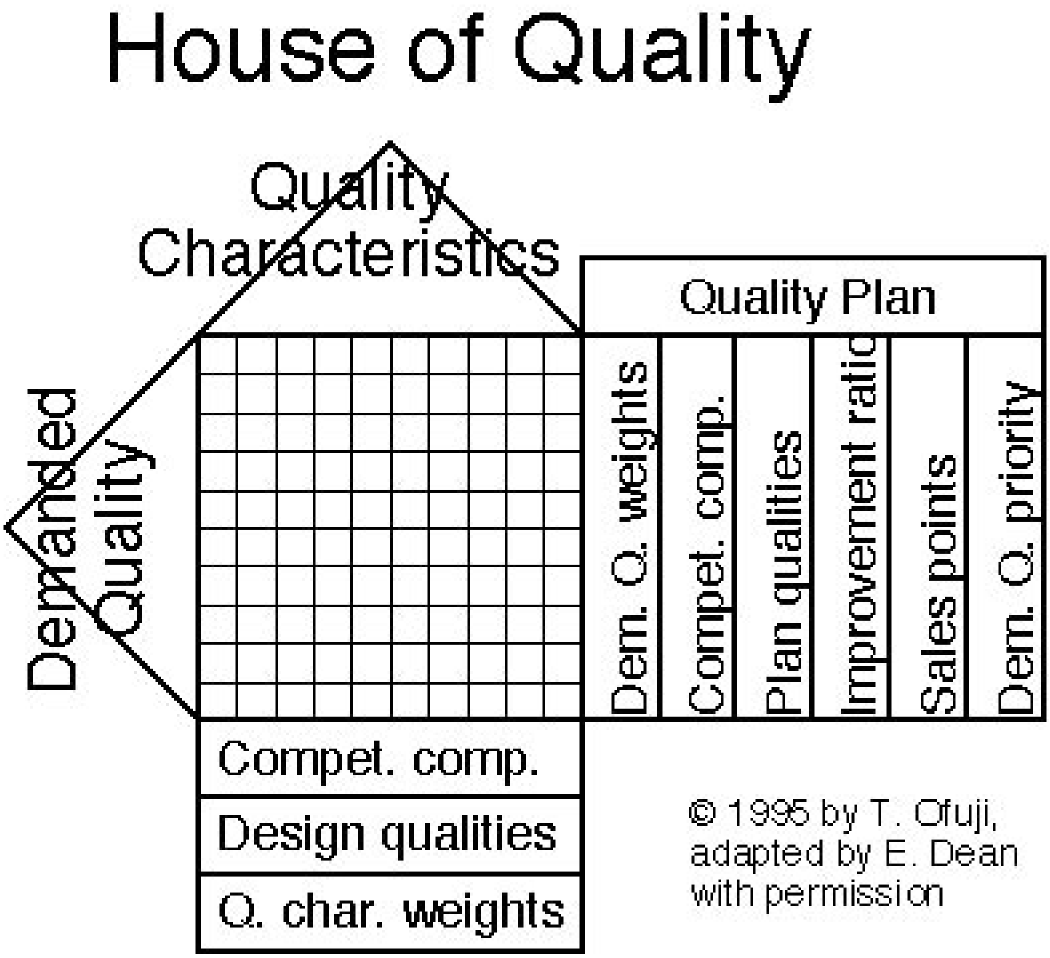
NIMROD

GROUND RULES

1. One vote per person
2. Decisions will be made by consensus
3. Avoid parochialism - work towards shared goal
4. Roles & responsibilities are clear, equitable and agreed to by all team members
5. Team members are willing to help one another
6. Keep everyone informed (open communication)
7. Mutual respect
8. Have fun
9. Meetings should have stated goals - set goal at end of meeting for next meeting.
10. Establish & adhere to a standard measuring stick for evaluations
11. Abstracts circulated before publication

QUALITY FUNCTION DEPLOYMENT (QFD)

"A method for developing a design quality aimed at satisfying the consumer and then translating the consumer's demand into design targets and major quality assurance points to be used throughout the production phase...[It] is a way to assure the design quality while the product is still in the design stage." - *Akao* (1990)



- **Translation of Customer Requirements into Design Requirements**
- **"Voice of the Customer" Heard at all Stages of Design and Development**
- **Avoid Re-Engineering after Product Deployment**

NIMROD CUSTOMERS

- ITER JOINT CENTRAL TEAM
- U.S. FUSION EXPERIMENTALISTS
- ALTERNATE CONCEPT DESIGNERS AND EXPERIMENTALISTS
- SYSTEM CODE DESIGNERS FOR TOKAMAKS

THE NIMROD EQUATIONS

Two-Fluid Equations ($\alpha = e,i$; $n_e = n_i = n$) :

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{v}_\alpha) = S_\alpha$$

$$m_\alpha n\left(\frac{\partial \mathbf{v}_\alpha}{\partial t} + \mathbf{v}_\alpha \cdot \nabla \mathbf{v}_\alpha\right) + \nabla p_\alpha + \nabla \cdot \Pi_\alpha = nq_\alpha\left(\mathbf{E} + \frac{1}{c}\mathbf{v}_\alpha \times \mathbf{B}\right) + \mathbf{R}_{\alpha,\beta}$$

$$\frac{3}{2}\left(\frac{\partial p_\alpha}{\partial t} + \mathbf{v}_\alpha \cdot \nabla p_\alpha\right) + \frac{5}{2}p_\alpha \nabla \cdot \mathbf{v}_\alpha + \nabla \cdot \mathbf{q} + \Pi_\alpha : \nabla \mathbf{v}_\alpha = Q_\alpha$$

$$p_\alpha = nk_B T_\alpha$$

Maxwell's Equations:

$$\nabla \cdot \mathbf{B} = \nabla \times \mathbf{E} + \frac{1}{c}\frac{\partial \mathbf{B}}{\partial t} = 0$$

$$\mathbf{B} = \nabla \times \mathbf{A} \qquad \mathbf{E} = -\nabla\phi - \frac{1}{c}\frac{\partial \mathbf{A}}{\partial t}$$

$$\nabla \times \nabla \times \mathbf{A} = \frac{4\pi}{c}\mathbf{J} + \frac{1}{c}\frac{\partial \mathbf{E}}{\partial t} \qquad \nabla \cdot \mathbf{J} = 0$$

Constitutive Equations:

$$\mathbf{J} = \sum_\alpha \mathbf{J}_\alpha = n\sum_\alpha q_\alpha \mathbf{v}_\alpha$$

Transport:

$$\mathbf{q}_\alpha = -\chi_{\perp\alpha}\nabla T_\alpha - (\chi_{\parallel\alpha} - \chi_{\perp\alpha})\hat{\mathbf{b}}\hat{\mathbf{b}} \cdot \nabla T_\alpha$$

$$\Pi_\alpha^{\text{viscous}} = -\nu_\alpha\left(\nabla \mathbf{v}_\alpha + \nabla \mathbf{v}_\alpha^{\mathrm{T}} - \frac{2}{3}\nabla \cdot \mathbf{v}_\alpha \mathbf{I}\right)$$

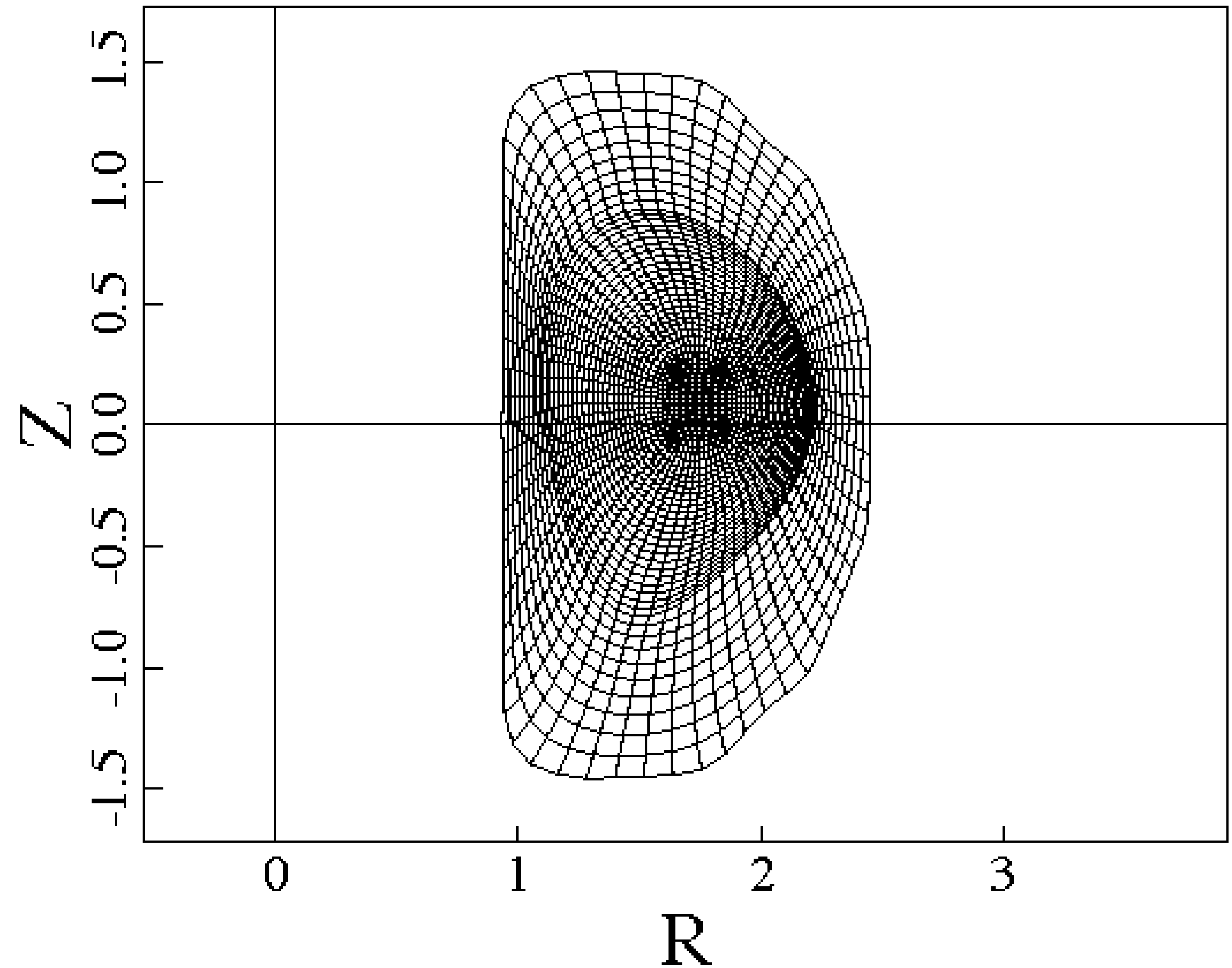
$$\Pi_\alpha^{\text{neo}} \approx \Pi_{\parallel\alpha}^{\text{neo}} = \left(\hat{\mathbf{b}}\hat{\mathbf{b}} - \frac{1}{3}\mathbf{I}\right)(p_\parallel - p_\perp)_\alpha$$

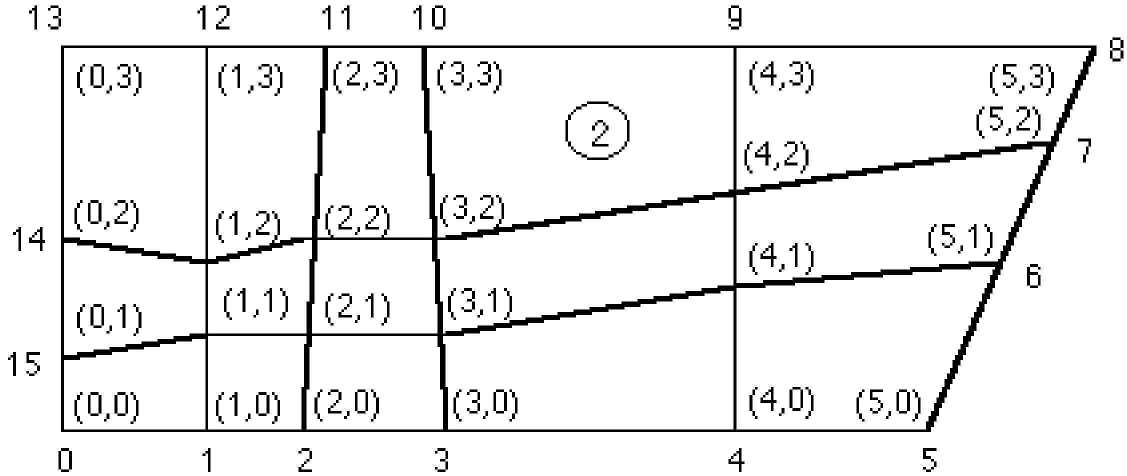
$$(p_\parallel - p_\perp)_\alpha = -m_\alpha n\mu_\alpha \frac{\langle B^2 \rangle}{\left\langle \left(\hat{\mathbf{b}} \cdot \nabla B\right)^2 \right\rangle}\mathbf{v}_\alpha \cdot \nabla \ln B$$

THE NIMROD GRID

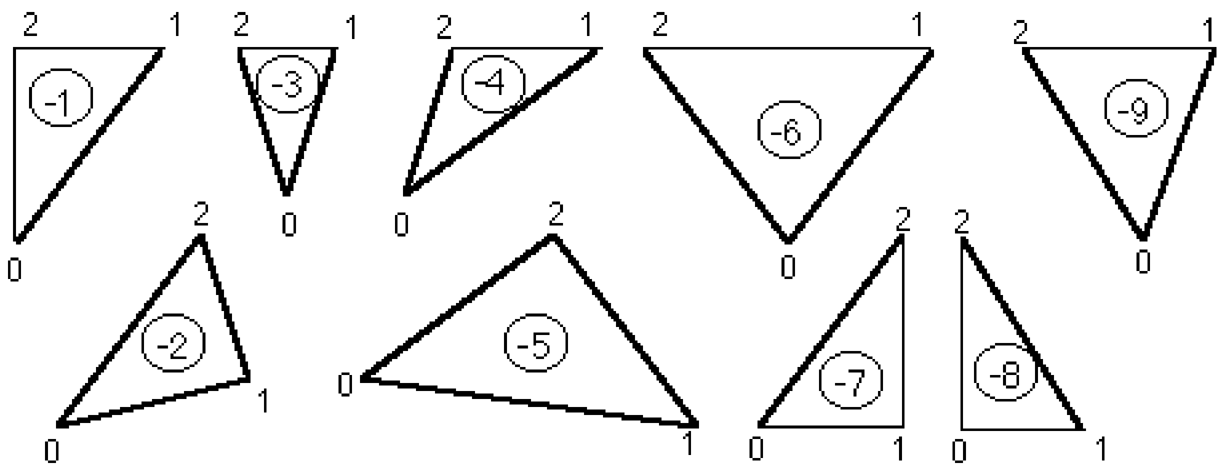
- Structured Grid in Toroidal Direction (Pseudospectral)
- Unstructured Blocks of Structured Quadrilaterals in Poloidal Plane
- Each Unstructured Block may be a Single Triangle (Patching of Non-Conforming Blocks)
- Outer Boundary can conform to Real Machine Geometry
- Nearly Flux Surface Conforming within Separatrix (Accuracy)
- Overlying Quadrilateral Grid near Magnetic Axis (Avoid Coordinate Singularity)
- Non-Orthogonal, Curvilinear Coordinates

Nimrod Grid (Equal Arc)

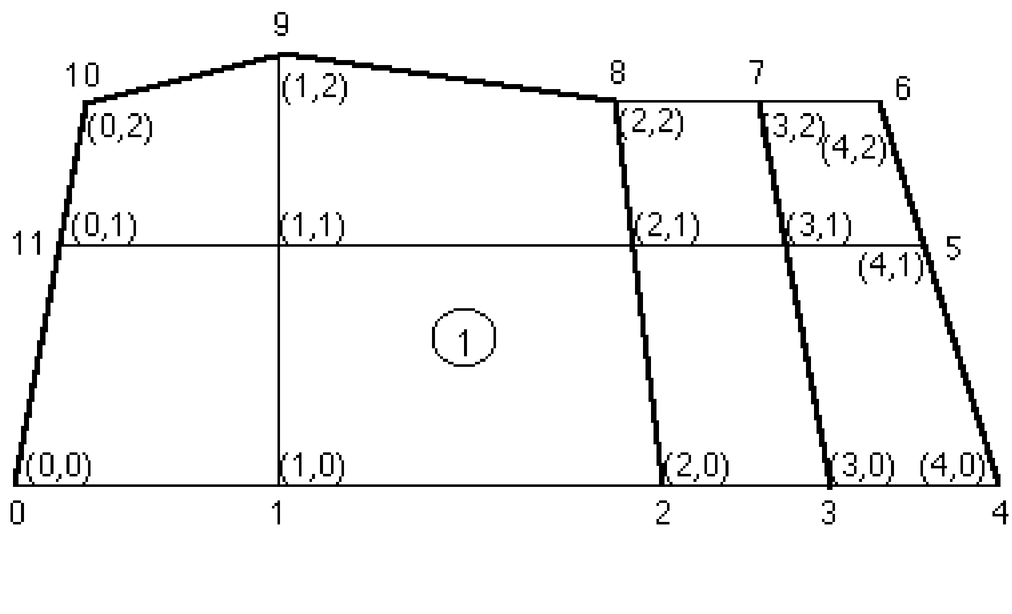




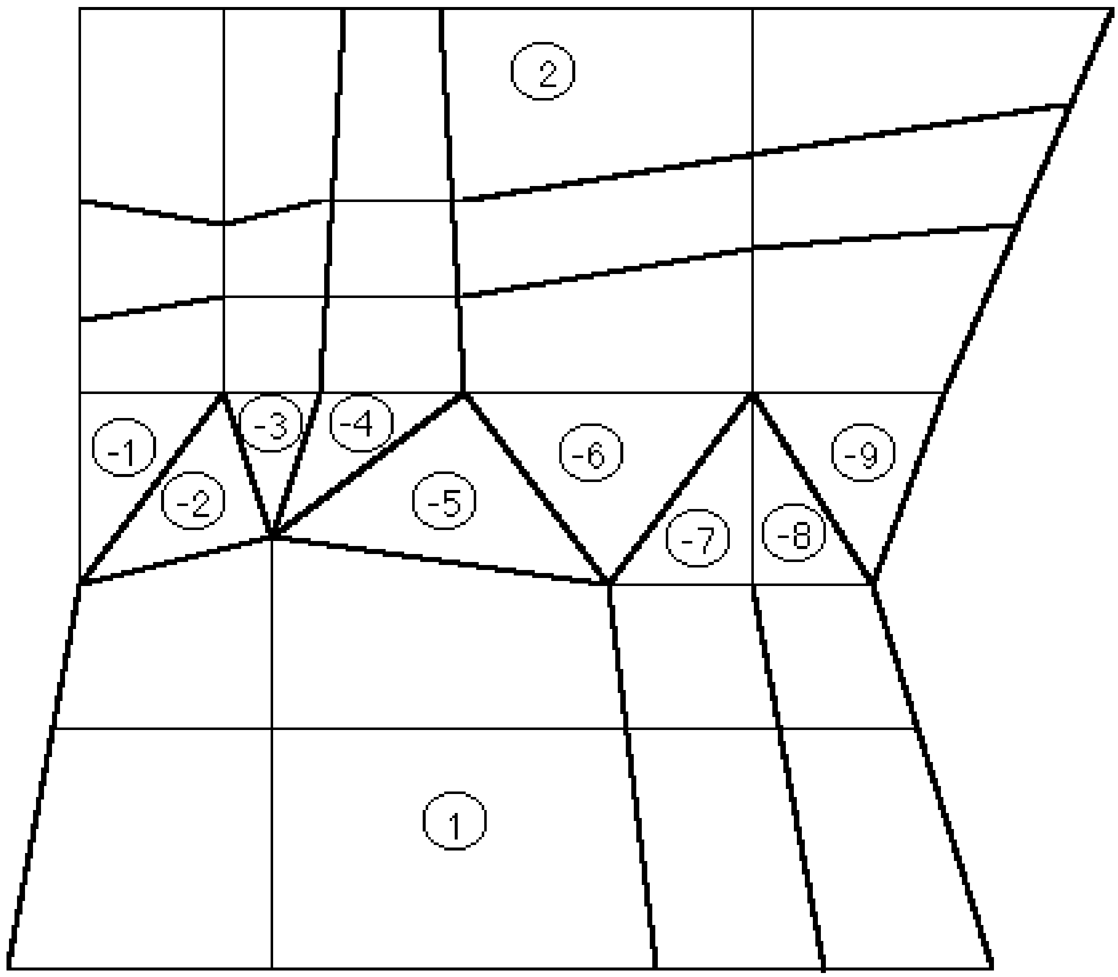
13
12
11
10
9
8
(0,3)
(1,3)
(2,3)
(3,3)
2
(4,3)
(5,3)
(5,2)
7
(4,2)
14
(0,2)
(1,2)
(2,2)
(3,2)
(5,1)
6
(4,1)
(0,1)
(1,1)
(2,1)
(3,1)
15
(0,0)
(1,0)
(2,0)
(3,0)
(4,0)
(5,0)
0
1
2
3
4
5



-1
-3
-4
-6
-9
-2
-5
-7
-8



9
10
8
7
6
(1,2)
(0,2)
(2,2)
(3,2)
(4,2)
11
(0,1)
(1,1)
(2,1)
(3,1)
5
(4,1)
1
(0,0)
(1,0)
(2,0)
(3,0)
(4,0)
0
1
2
3
4



2
-1
-2
-3
-4
-5
-6
-7
-8
-9
1

NONORTHOGONAL, CURVILINEAR COORDINATES FOR POLOIDAL PLANE

- **Coordinate Transformation:**

$$R = R(\xi, \eta) \qquad Z = Z(\xi, \eta)$$

$$\mathbf{e}_i = \frac{\partial \mathbf{r}}{\partial q^i}, \qquad q^i = (\xi, \eta), \qquad g_{ij} = \mathbf{e}_i \cdot \mathbf{e}_j$$

- **Jacobian:**

$$J = R\sqrt{g_{\xi\xi} g_{\eta\eta} - g_{\xi\eta}^2}$$

- **Reciprocal Basis:**

$$\mathbf{e}^\xi = J^{-1}\mathbf{e}_\eta \times \mathbf{e}_\phi, \qquad \mathbf{e}^\eta = J^{-1}\mathbf{e}_\phi \times \mathbf{e}_\xi, \qquad \mathbf{e}^\phi = \mathbf{e}_\phi$$

$$g^{\xi\xi} = \frac{R^2}{J^2} g_{\eta\eta}, \qquad g^{\xi\eta} = -\frac{R^2}{J^2} g_{\xi\eta}, \qquad g^{\eta\eta} = \frac{R^2}{J^2} g_{\xi\xi}$$

- **Scalar Product:**

$$\mathbf{A} \cdot \mathbf{B} = g^{\xi\xi} A_\xi B_\xi + g^{\xi\eta}\left(A_\xi B_\eta + A_\eta B_\xi\right) + g^{\eta\eta} A_\eta B_\eta + A_\phi B_\phi$$

- **Vector Product:**

$$(\mathbf{A} \times \mathbf{B})^\xi = \frac{R}{J}\left(A_\eta B_\phi - A_\phi B_\eta\right), \quad (\mathbf{A} \times \mathbf{B})^\eta = \frac{R}{J}\left(A_\phi B_\xi - A_\xi B_\phi\right), \quad (\mathbf{A} \times \mathbf{B})_\phi = \frac{R}{J}\left(A_\xi B_\eta - A_\eta B_\xi\right)$$

- **Divergence:**

$$\nabla \cdot \mathbf{A} = \frac{1}{J}\left[\frac{\partial}{\partial \xi} J\left(g^{\xi\xi} A_\xi + g^{\xi\eta} A_\eta\right) + \frac{\partial}{\partial \eta} J\left(g^{\xi\eta} A_\xi + g^{\eta\eta} A_\eta\right)\right] + \frac{n}{R} A_\phi$$

- **Curl:**

$$(\nabla \times \mathbf{A})^\xi = \frac{i}{J}\left(\frac{\partial}{\partial \eta} RA_\phi + nA_\eta\right), \quad (\nabla \times \mathbf{A})^\eta = -\frac{i}{J}\left(\frac{\partial}{\partial \xi} RA_\phi + nA_\xi\right), \quad (\nabla \times \mathbf{A})_\phi = \frac{iR}{J}\left(\frac{\partial A_\xi}{\partial \eta} - \frac{\partial A_\eta}{\partial \xi}\right)$$

NIMROD TIME ADVANCE

- **Ion and Electron Currents (Momenta) and Electric Field Advanced Implicitly and Simultaneously**

- **Predictor-Corrector Iterations**

$$\mathbf{J}_\alpha^{n+1} = \mathbf{J}_\alpha^* + \delta\mathbf{J}_\alpha, \quad \mathbf{E}^{n+1} = \mathbf{E}^* + \delta\mathbf{E}$$

- **Correctors $\delta\mathbf{E}$ and $\delta\mathbf{J} = \delta\mathbf{J}_e + \delta\mathbf{J}_i$ related by**

$$\frac{4\pi\Delta t}{c^2}\delta\mathbf{J} = \mathbf{S}\cdot\delta\mathbf{E}$$

$$\mathbf{S} = S_\parallel \hat{\mathbf{b}}\hat{\mathbf{b}} + S_\perp\left(\mathbf{I} - \hat{\mathbf{b}}\hat{\mathbf{b}}\right)$$

$$S_\parallel = \frac{f_E \sum_\alpha \frac{\omega_{p\alpha}^2 \Delta t^2}{c^2}}{1 + \frac{\eta f_\eta c^2}{4\pi\Delta t}\sum_\alpha \frac{\omega_{p\alpha}^2\Delta t^2}{c^2}}, \qquad S_\perp = \frac{f_E \sum_\alpha \frac{\omega_{p\alpha}^2 \Delta t^2 / c^2}{1 + f_\Omega^2 r_\alpha^2}}{1 + \frac{\eta f_\eta c^2}{4\pi\Delta t}\sum_\alpha \frac{\omega_{p\alpha}^2\Delta t^2 / c^2}{1 + f_\Omega^2 r_\alpha^2}}$$

- **Implicit Equation for $\delta\mathbf{E}$:**

$$f_E \Delta t^2 \nabla\times\nabla\times\delta\mathbf{E} + \mathbf{S}\cdot\delta\mathbf{E} = -\frac{\Delta t}{c}\left(\nabla^2\mathbf{A}^* + \frac{4\pi}{c}\mathbf{J}^*\right)$$

- **Correctors go to Zero as Iterations Converge**

- **Viscosity Advanced by Operator Splitting**

- **Semi-Implicit Advance for Pressure and Density**

NIMROD SPATIAL DIFFERENCING

- **Finite Element Formulation:**

$$R(\xi,\eta)=\sum_{i,j}\hat{R}_{i,j}s_{i,j}(\xi,\eta), \qquad Z(\xi,\eta)=\sum_{i,j}\hat{Z}_{i,j}s_{i,j}(\xi,\eta),$$

$$f(\xi,\eta,\phi,t)=\sum_{n}e^{in\phi}\sum_{i,j}\hat{f}^{n}_{i,j}(t)w_{i,j}(\xi,\eta)$$

- **Difference Equations Derived from Variational Principle:**

$$\frac{f_E\Delta t^2}{2}\int d\mathbf{r}\left[(\nabla\cdot\delta\mathbf{E})^2+(\nabla\times\delta\mathbf{E})^2\right]+\frac{1}{2}\int d\mathbf{r}\delta\mathbf{E}\cdot\mathbf{S}\cdot\delta\mathbf{E}$$

$$=\int d\mathbf{r}\left[(\nabla\cdot\delta\mathbf{E})(\nabla\cdot\delta\mathbf{A}^*)+(\nabla\times\delta\mathbf{E})\cdot(\nabla\times\delta\mathbf{A}^*)\right]$$

$$-\frac{4\pi\Delta t^2}{c^2}\int d\mathbf{r}\delta\mathbf{E}\cdot\mathbf{J}^*$$

- **Example: Scalar Laplacian**

$$\int d\mathbf{r}\delta\phi\nabla_{\mathrm{P}}^2\phi=-\frac{1}{2}\delta\int d\mathbf{r}\left|\nabla_{\mathrm{P}}\phi\right|^2$$

$$\sum_{p,q}\delta\phi_p\left[M_{p,q}\left(\nabla_{\mathrm{P}}^2\phi\right)_q-G_{p,q}\phi_q\right]=0, \qquad p=(i,j), \qquad q=(i',j')$$

$$\mathbf{M}\cdot\nabla_{\mathrm{P}}^2\phi=\mathbf{G}\cdot\phi$$

$$M_{p.q}=\int d\xi d\eta Jw_p(\xi,\eta)w_q(\xi,\eta)$$

$$G_{p,q}=-\int d\xi d\eta J\nabla w_p(\xi,\eta)\cdot\nabla w_q(\xi,\eta)=$$

$$-\int d\xi d\eta J\left[g^{\xi\xi}\frac{\partial w_p}{\partial\xi}\frac{\partial w_q}{\partial\xi}+g^{\xi\eta}\left(\frac{\partial w_p}{\partial\xi}\frac{\partial w_q}{\partial\eta}+\frac{\partial w_p}{\partial\eta}\frac{\partial w_q}{\partial\xi}\right)+g^{\eta\eta}\frac{\partial w_p}{\partial\eta}\frac{\partial w_q}{\partial\eta}\right]$$

NIMROD STATUS

- NIMROD Tasks Defined
- Software Standards Defined
  - Parallel Computing Paradigm
  - High Level Modules and Interfaces (C++, Python, Tcl/Tk)
  - Physics Modules (Fortran 90)
- Flowcharts and Documentation Produced
- Grid Generator Implemented and Tested
- NIMROD Version 0.2
  - Cold Plasma
  - Alfvén waves (implicit)
  - Interfaced with full grid
- Pre-processor, Post-processor and GUI Written
  - Equilibrium, Grid, and Input Generation
  - NIMROD Execution
  - Graphical Animation
- Parallel Computing Issues Being Studied
  - CG solver
  - Code structure
- NIMROD Schedule:
  - Initial Demonstration Nov. 1996 (APS)
  - First Product Delivery (beta-test version to GA) July 1997
  - Full Production Version July 1998
- On Schedule

SOFTWARE STANDARDS FOR NIMROD

Report 2.1
September 27, 1996

1. LANGUAGES

We will write the computationally intensive mathematics and physics kernels in F90. Programmers should at all time write simple, clear, parallel (loop bodies are independent) code. Parallel loops should be identified with an appropriate comment. The comment will make it easy to insert the appropriate pragma. if necessary, and facilitate conversion to HPF whan compilers mature.

When using the module containing global data, specify which variables are imported.

2. I/O

The code will write restart files every n time steps. This will be the preferred way to start or restart NIMROD. The pre-processor will generate a restart file containing the initial data. We will allow user customized files to be output at user defined timesteps. The current input files will be saved (Ming/Olivier/Alan T. to claify.).

After discussion on 25 September 1996 at the Germantown NIMROD meeting, netcdf has been dropped from the software standards and in the interim replaced with binary fortran reads and writes.

In review the primary advantages for netcdf were:

1) Self describing.
2) Portable across platforms.

The primary disadvantages were:

1) Incomptable with the structures/derived types of f90.
2) Output files larger by a factor of 2 to 3 over straight f90 binary. [This is the previous version deleted as of 9/26/97: The proposed file format is netcdf. This manager works on several platforms including the T3D and is compatible with IDL. If experience shows netcdf is inappropriate or better packages are available, we may revisit this decision. Once the difinitive choice is made, we will develop the program/database interface so that developers can use the database for testing prruposes.]

3. PROGRAMMING STANDARDS

We will write LP code with comments where MP routines can be inserted for conversion to an MPP platform. We will use free-format Fortran 90 with level indentation . Space will be left at the beginning of lines for statement labels. We will use "&" for continuation, and "!" for comments.

1. General Comments

   No common blocks.
   No include files.
   Interface modules to be written for external libraries.
   All public global data is isolated to a single global module.
   Modules and subroutines retain no state.
   No equivalence statements.
   No aliases (a name is passed only once to a subroutine).
   No pointer-to-pointer assignments: `p => a`. (Only `p=a` is allowed.)

2. All subroutines must include the statement "`implicit none`". (Use strong typing).

   Programmers are encouraged, as readability permits, to start integer and boolean names with the letters [i,n], complex names with c, and real names with other letters.

3. Comments:

   Declare INTENT of all formal parameters.
   Include comments within the module.

4. Code in F90 free-format.

   Use level indentation.
   Allow space at the beginning of lines for statement labels.
   Use "&" for continuation.
   Use "!" for comment.

5. Use the following type definitions(defined in single system module:

```
real(real8) = r8
integer(integer4) = I4
complex(complex16) = C16
logical(logical4) = L4
```

6. Explicitely specify type when passing constants through an argument list:

```
2.34_real8 4_integer4
```

7. Break proceedures into sub-proceedures if the same functionality isused several times, but be reasonable.

8. For exiting the program, use "`call EXIT_NIMROD(string)`", for example.

4. SOFTWARE MAINTENANCE

We propose to use CVS for software maintenance (pending a report from Jim Crottinger).

5. LIBRARIES

We will not adopt special libraries with the exception of the standard C and Fortran math libraries. If someone wishes to include modules from a library package (such as BLAS2/BLAS3), they should petition the NIMROD working group and make their case. The group will the reach a concensus decision regarding the use of the library.

6. SCRIPT AND GUI LANGUAGES

We will use PYTHON as the script language to interface system components, such as the pre-and post-processors. The persons responsible for developing the GUI may choose the GUI language of their choice; it must be compatible with C++ and PYTHON. At this time, we recommend tk.

7. GRAPHICS

XDRAW will be used until the November, 1996, APS Meeting. (Alan Glasser is to explore other possibilities.) IBM Data Explorer is now being used, also.

NIMROD VALIDATION PLAN

(DRAFT 9/20/96 Rev. 1)

I. Stable linear oscillations (MHD limit only)

A. Uniform Bphi, no current

1. Zero beta, 2-D

a. Compressional Alfven waves, plasma oscillations, whistler waves, all cases have perfectly conducting boundary on plasma

i) Rectangular region - frequency known analytically

* Uniform grid

- Explicit

- Implicit

* Non uniform grid

- Explicit

- Implicit

ii) Cylindrical region

* Multiple blocks with seams

2. Zero beta, 3-D

a. Compressional Alfven waves, plasma oscillations, whistler waves - n=0
-Repeat the above test to assure there are no surprises.

b. Torsional Alfven waves, n > 0 - Compare frequency with analytic (?) solutions and with GATO. (Initialize with GATO eigenfunction?) Both explicit and implict cases.

i) Single block grid

ii) Multiple block grid with seams

3. Finite beta, 2-D

a. Electron sound waves (turn off ions)
b. Ion sound waves (both species on)
c. Drift waves

4. Finite beta, 3-D redo 2-D cases

B. Force-free toroidal equilibria - Comparision with GATO frequencies and eigenfunctions.

I. Linear unstable modes, 3D (Ideal MHD limit)

A. Internal modes (perfectly conducting boundary at separatrix).

1. Force-free toroidal equilibria (are there any that we understand?)

2. Finite beta

a. Solov'ev equilibrium - Internal kink modes

i) Berger, et al, paper (growth rates and eigenfunctions)

ii) comparison of marginal points with Berger, et al., and DCON

b. Numerical equilibria - Compare growth rates and eigenfunctions with GATO, Keldish codes, marginal points with DCON

i) DIIID

ii) TFTR

iii) ITER

iv) etc, etc, etc........

B. External modes - vacuum region - Comparisons with GATO.

II. Linear unstable modes (Resistive MHD)

A. Compare with Carreras, et al (n = 2 tearing mode in a circular cross section torus) - Growth rate and eigenfunction

B. Any other known toroidal solutions (Keldish codes?)
C. Marginal points (DCON?)

IV. Linear unstable modes with 2-Fluid effects

A. Cylindrical case (Pic3d comparison)

1. Ideal (1,1) mode

2. Resistive (2,1) mode

B. Toroidal case (QIP3D comparison)

1. Resistive (1,1) mode

2. Resistive (2,1) mode

V. Nonlinear evolution (Ideal and resistive MHD) - We need to identify a suite of nonlinear problems with known solutions, either from the published literature or in collaboration with other 3-D nonlinear codes.

A. Internal modes???

B. External modes (requires moving separatrix)???

VI. Thermal Conductivity - Test pollution of perpindicular transport in highly anisotropic cases. Impose islands and see how well temperature conforms to the flux surfaces.

VII. Nonlinear evolution with 2-Fluid effects

A. Cylindrical case (Pic3d comparison)

1. Ideal (1,1) mode

2. Resistive (2,1) mode

B. Toroidal case (QIP3D comparison)

1. Resistive (1,1) mode

2. Resistive (2,1) mode

VIII. Neo-Classical effects - We need to define a suite of test problems

IX. Comparison with experiment