AN OVERVIEW OF THE NIMROD CODE

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and
The NIMROD Team

OUTLINE

- **What is NIMROD?**
  - The NIMROD project
  - The NIMROD code system
- **The NIMROD physics kernel**
  - The 2-fluid equations
  - The implicit field equation (cold plasma)
  - Warm plasma effects++
  - The NIMROD grid
- **Implementation**
  - Programming standards
  - GUI
  - Graphics
  - Parallel computing
- **Status and plans**

WHAT IS NIMROD?

- **AN ACRONYM:**
  - **Non-Ideal MHD with Rotation: Open Discussion**
- **A CODE:**
  - **To simulate non-ideal, 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!

First meeting: February, 1996

THE NIMROD TEAM

Curt Bolton	DOE/OFE	Scott Kruger	U. Wisc.
Ming Chu	GA	Rick Nebel	LANL
Paul Covello	LLNL	Steve Plimpton	SNL (ABQ)
Jim Crotinger	LLNL	Nina Popova	Moscow St. U.
Sergei Galkin	Keldysh Inst.	Olivier Sauter	ITER
Tom Gianakon	Cadarache	Dalton Schnack	SAIC
Alan Glasser	LANL	Carl Sovinec	LANL
Shri Gopaladrishna	LLNL	Alfonso Tarditi	SAIC
Harsh Karandakar	SAIC	Alan Turnbull	GA
Alice Koniges	LLNL		

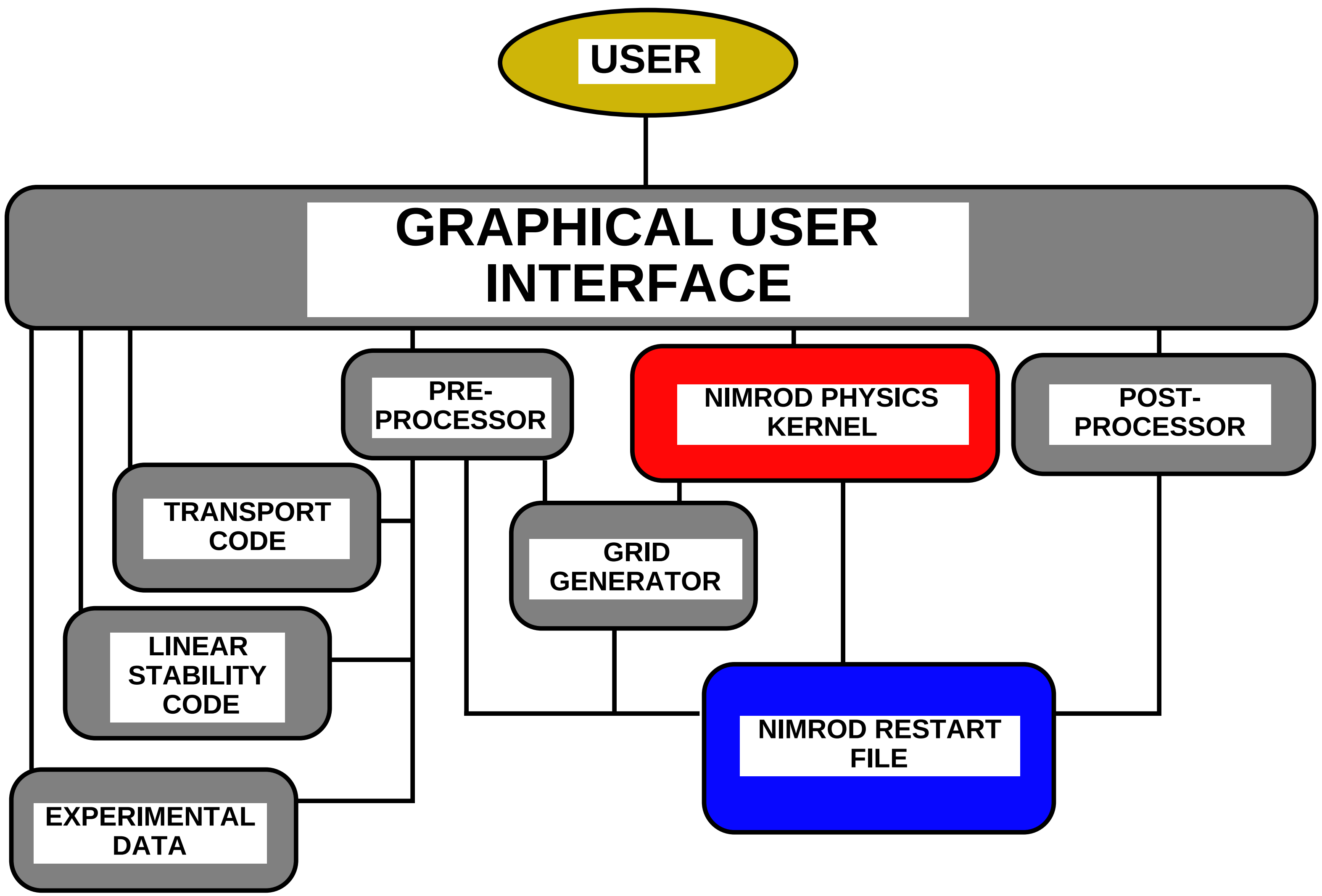
NIMROD IS A COMPUTATIONAL INITIATIVE

- **Collaboration with MICS**
  - Linear solver
    - SNL/ABQ
    - LLNL
  - Parallel computing issues
    - SNL/ABQ
    - NERSC
  - Remote operation
    - NERSC
- **Spinoff to the fusion program**
  - GUI
    - Used at GA
  - Free, high quality graphics (XDRAW)
- **Development of team techniques**
  - Remote, multi-institutional code development project

THE NIMROD CODE SYSTEM

- **Driven by GUI**
  - **NIMROD**
  - **User defined codes**
  - **Monitor and interact with jobs**
- **Pre-processor**
  - **Defines problem**
    - **Geometry**
    - **Initial conditions**
    - **Grid**
  - **Interacts with user-defined files**
    - **Equilibrium, transport, stability codes**
    - **Experimental data**
    - **Standard file formats**
- **NIMROD physics kernel**
  - **Initial/boundary value problem**
  - **2-fluid equations**
  - **Generates interim output**
- **Post-processor**
  - **"Quick-look" graphics**
    - **XDRAW**
  - **Animation, advanced graphics**
    - **DX**
  - **Interface with commercial software**
    - **HDF files, etc.**
  - **User-defined diagnostics**

THE NIMROD CODE SYSTEM



THE NIMROD PHYSICS KERNEL

Faraday and Ampere:

$$\frac{1}{c}\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} \qquad \nabla \times \mathbf{B} = \frac{4\pi}{c}\mathbf{J} + \frac{1}{c}\frac{\partial \mathbf{E}}{\partial t}$$

Equation of motion (α = *e*,*i*; $n_e = Zn_i = n$):

$$m_\alpha n_\alpha \left(\frac{\partial \mathbf{v}_\alpha}{\partial t} + \mathbf{v}_\alpha \cdot \nabla \mathbf{v}_\alpha \right) = -\nabla \cdot \Pi_\alpha + q_\alpha n_\alpha \left(\mathbf{E} + \frac{1}{c}\mathbf{v}_\alpha \times \mathbf{B} \right) + \sum_\beta \mathbf{R}_{\alpha\beta} + \mathbf{S}_\alpha^m$$

Thermodynamics:

$$\frac{\partial p_\alpha}{\partial t} + \mathbf{v}_\alpha \cdot \nabla p_\alpha = -\frac{3}{2} p_\alpha \nabla \cdot \mathbf{v}_\alpha - \Pi_\alpha : \nabla \mathbf{v}_\alpha - \nabla \cdot \mathbf{q}_\alpha + \mathbf{Q}_\alpha$$

Continuity:

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

Auxiliary equations:

$$p_\alpha = n_\alpha k_B T_\alpha \qquad \mathbf{J} = \sum_\alpha \mathbf{J}_\alpha = \sum_\alpha n_\alpha q_\alpha \mathbf{v}_\alpha \qquad \mathbf{M} = \sum_\alpha \mathbf{M}_\alpha = \sum_\alpha m_\alpha \mathbf{J}_\alpha / q_\alpha$$

IMPLICIT FIELD EQUATION

- **Cold plasma** $\Rightarrow$ $p_\alpha = 0, \qquad n = const.$
- **Low frequency** $\Rightarrow$ **Ignore displacement current**

$$\frac{\partial \mathbf{J}_\alpha}{\partial t} + \frac{q_\alpha}{m_\alpha c}\mathbf{B}\times\mathbf{J}_\alpha = \frac{nq_\alpha^2}{m_\alpha}\mathbf{E} \qquad \frac{\partial \mathbf{M}_\alpha}{\partial t} = q_\alpha n\mathbf{E} + \frac{1}{c}\mathbf{J}_\alpha \times \mathbf{B}$$

- **Time differencing, sum over species:** $\mathbf{J}_\alpha^{n+1} = \mathbf{J}_\alpha^n + \Delta\mathbf{J}_\alpha, \quad 0 < f_\Omega \le 1$**,** $\omega_p^2 = \omega_e^2 + \omega_i^2$**,** $\omega_\alpha^2 = 4\pi n q_\alpha^2 / m_\alpha$

$$\frac{\Delta\mathbf{J}}{\Delta t} + f_\Omega \frac{1}{c}\mathbf{B}\times\sum_\alpha \frac{q_\alpha}{m_\alpha}\mathbf{J}_\alpha^{n+1} = \frac{\omega_p^2}{4\pi}\mathbf{E} + (f_\Omega - 1)\frac{1}{c}\mathbf{B}\times\sum_\alpha \frac{q_\alpha}{m_\alpha}\mathbf{J}_\alpha^n$$

$$\frac{\Delta\mathbf{M}}{\Delta t} = \frac{1}{c}\left(f_\Omega \Delta\mathbf{J} + \mathbf{J}^n\right)\times\mathbf{B}$$

- **A useful expression:** $\nu = Zm_e / m_i, \quad q_e = -e, \quad q_i = Ze$

$$\sum_\alpha \frac{q_\alpha}{m_\alpha}\mathbf{J}_\alpha = \frac{Ze^2}{m_i m_e}\mathbf{M} - \frac{e}{m_e}(1-\nu)\mathbf{J}$$

IMPLICIT FIELD EQUATION (cont.)

- **Solve for E (generalized Ohm's law)** $\rho = mn, \quad m = m_e + m_i / Z$

$$\mathbf{E} = \mathbf{E}_{im} + \mathbf{E}_{ex}$$

$$\mathbf{E}_{im} = \underbrace{\frac{4\pi}{\omega_p^2}\frac{\Delta\mathbf{J}}{\Delta t}}_{Inertia} + \underbrace{\frac{f_\Omega^2 \Delta t}{\rho c^2}\left(B^2\mathbf{I} - \mathbf{BB}\right)\cdot\Delta\mathbf{J}}_{MHD} - \underbrace{\frac{1-\nu}{1+\nu}\frac{f_\Omega}{nec}\mathbf{B}\times\Delta\mathbf{J}}_{Hall}$$

$$\mathbf{E}_{ex} = \frac{1}{\rho c}\left[\mathbf{B}\times\mathbf{M}^n + \frac{f_\Omega \Delta t}{c}\left(B^2\mathbf{I} - \mathbf{BB}\right)\cdot\mathbf{J}^n\right] - \frac{1-\nu}{1+\nu}\frac{1}{nec}\mathbf{B}\times\mathbf{J}^n$$

- **Impedance tensor,** $\mathbf{E}_{im} = (4\pi / c)\mathrm{Z}\cdot\Delta\mathbf{J}$**:**

$$\mathrm{Z} = c\Delta t\left\{\frac{1}{\left(\omega_p \Delta t\right)^2}\hat{\mathbf{b}}\hat{\mathbf{b}} + \left[\frac{1}{\left(\omega_p \Delta t\right)^2} + f_\Omega^2\left(\frac{V_A}{c}\right)^2\right]\left(\mathbf{I} - \hat{\mathbf{b}}\hat{\mathbf{b}}\right) - \frac{1-\nu}{1+\nu}\frac{f_\Omega}{\Omega\Delta t}\left(\frac{V_A}{c}\right)^2\hat{\mathbf{b}}\times\mathbf{I}\right\}$$

- **Combine with Maxwell** $\Rightarrow$ **Implicit field equation:**

$$\boxed{\begin{gathered} c\Delta t\nabla\times\mathrm{Z}\cdot\nabla\times\Delta\mathbf{B} + \Delta\mathbf{B} = -c\Delta t\nabla\times\mathbf{E}_{ex} \\ \Delta\mathbf{B} = \mathbf{B}^{n+1} - \mathbf{B}^n \end{gathered}}$$

IMPLICIT FIELD EQUATION

- **Must invert operator**

$$\Omega = \mathbf{I} + c\Delta t \nabla \times \mathsf{Z} \cdot \nabla \times \mathbf{I}$$

- $\mathsf{Z} = \mathsf{Z}_S + \mathsf{Z}_A$**, where is symmetric and**

$$\mathsf{Z}_A = c\Delta t \frac{1-\nu}{1+\nu} \frac{f_\Omega}{\Omega \Delta t} \left(\frac{V_A}{c} \right)^2 \hat{\mathbf{b}} \times \mathbf{I}$$

- **Symmetric part of $\Omega = \mathbf{S} + \mathbf{A}$ is positive definite**

$$\delta I = 0, \qquad I = \frac{1}{2} \int d\mathbf{x} \left\{ \left| \Delta \mathbf{B} \right|^2 + c\Delta t \left[(\nabla \times \Delta \mathbf{B}) \cdot \mathbf{S} \cdot (\nabla \times \Delta \mathbf{B}) \right] \right\}$$

- **Solve related symmetric system**

$$\left(\mathbf{S} + \mathbf{S}_A \right) \cdot \left(\Delta \mathbf{B}^{l+1} - \Delta \mathbf{B}^{l} \right) = -c\Delta t \nabla \times \mathbf{E}_{ex} - \Omega \cdot \Delta \mathbf{B}^{l}$$

  where $\mathbf{S}_A$ is symmetric positive definite "semi-implicit" operator

- $\|\mathbf{A}\| / \|\mathbf{S}\| \sim 1 / \Omega \Delta t << 1$ **for low frequency motions**

IMPLICIT FIELD EQUATION

- **CG matrix inversion for symmetric system**
  - Diagonal preconditioner
  - Block-direct preconditioner
  - Anti-symmetric part treated "semi-implicitly"
- **Unconditionally stable for arbitrary Δt**
  - Cold plasma waves
- **Advection**
  - Explicit $\Rightarrow$ $V\Delta t / \Delta x < 1$
- **Spatial discretization by finite elements**
  - Dependent variables: bi-linear elements
  - Metric elements: bi-cubic splines
- **No spectral pollution**
- **No "red-black" mode**
- **May require "divergence cleaning"**

WARM PLASMA EFFECTS++

- **Finite temperature (pressure)**
  - **Explicit pressure gradient in field equation**
  - **Energy equations solved in separate step**
    - **Semi-implicit advance stabilizes sound waves**
- **Continuity $\Rightarrow$ straightforward**
- **Heat conduction**
  - **Anisotropic thermal transport stabilized by semi-implicit operator**
- **Energetic species**
  - **Push particles, take moments**
- **Neoclassical stress tensor**

$$\nabla \cdot \Pi_\alpha^{\mathrm{neo}} = \mathbf{BB} \cdot \nabla\left(\frac{f_\alpha}{B^2}\right) + \frac{f_\alpha}{B^2}\nabla\left(\frac{B^2}{2}\right) - \frac{f_\alpha}{B^2}\mathbf{B}\times\nabla\times\mathbf{B} - \frac{1}{3}\nabla f_\alpha$$

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

- **Sources of momentum, mass, and energy**

TIME ADVANCE

- $Z = Z(\mathbf{B}, n, p_\alpha) \Rightarrow$ **Iteration required**

- **Inner iteration: solve**

$$c\Delta t \nabla \times Z(\mathbf{B}^l, n, p_\alpha) \cdot \nabla \times \Delta \mathbf{B}^{l+1} + \Delta \mathbf{B}^{l+1} = -c\Delta t \nabla \times \mathbf{E}_{ex}$$

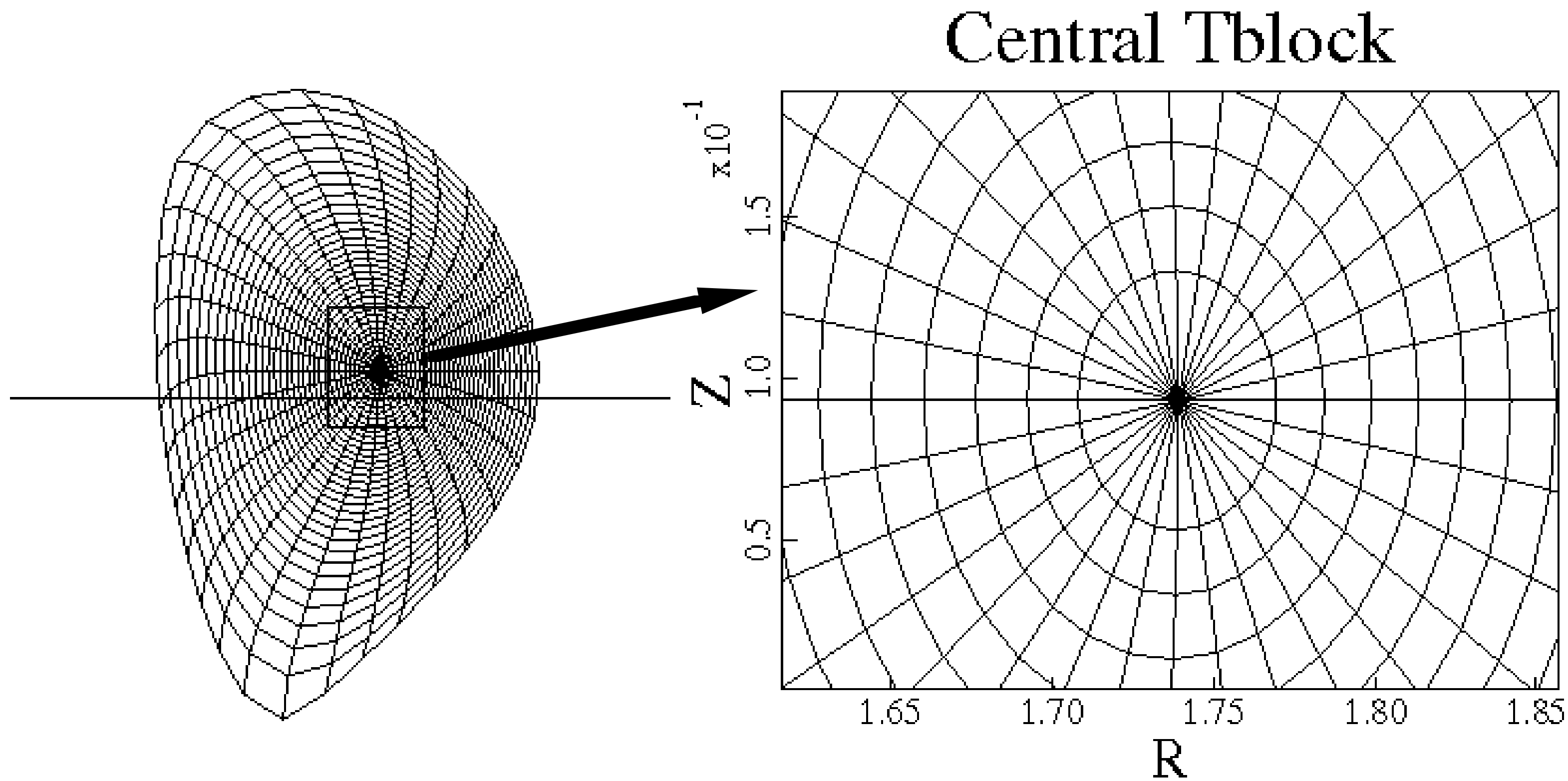
  until iterations for B converge

- **Outer iteration**
  - **advance energy and continuity equations**
  - **Update impedance tensor**
  - **Repeat field solve**

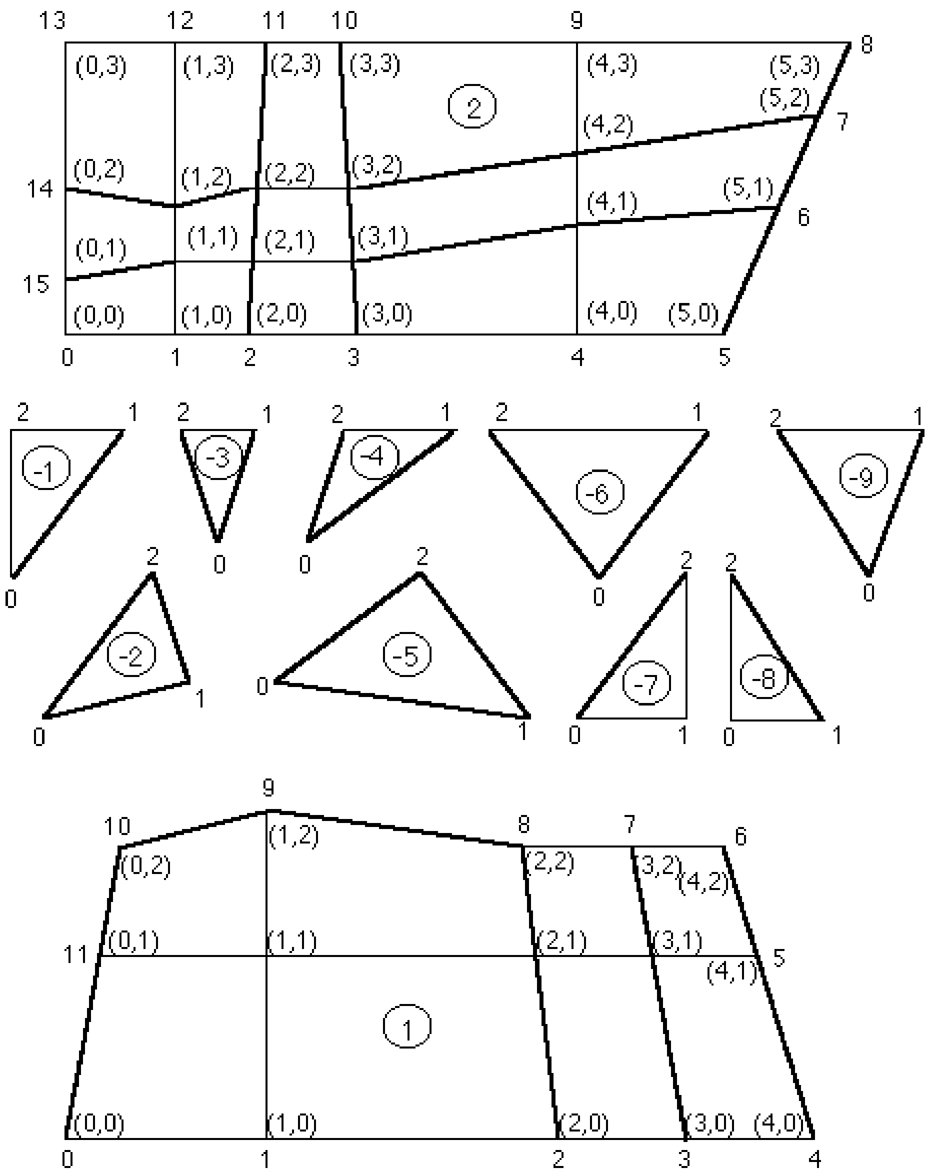
THE NIMROD GRID

- Structured grid in toroidal direction (Pseudospectral)
  - Fourier collocation
  - Dealiased
  - FFTs
- Unstructured blocks in poloidal plane
  - RBLOCKs
    - Structured quadrilaterals
  - TBLOCKs
    - Triangles
- Nonconforming RBLOCKs joined with TBLOCKs
- Outer Boundary can conform to real machine geometry
- Nearly flux surface conforming within separatrix (accuracy)
- TBLOCKS near magnetic axis (avoid coordinate singularity)
- Non-orthogonal, curvilinear coordinates

NIMROD GRID



JOINING NONCONFORMING RBLOCKs WITH TBLOCKs



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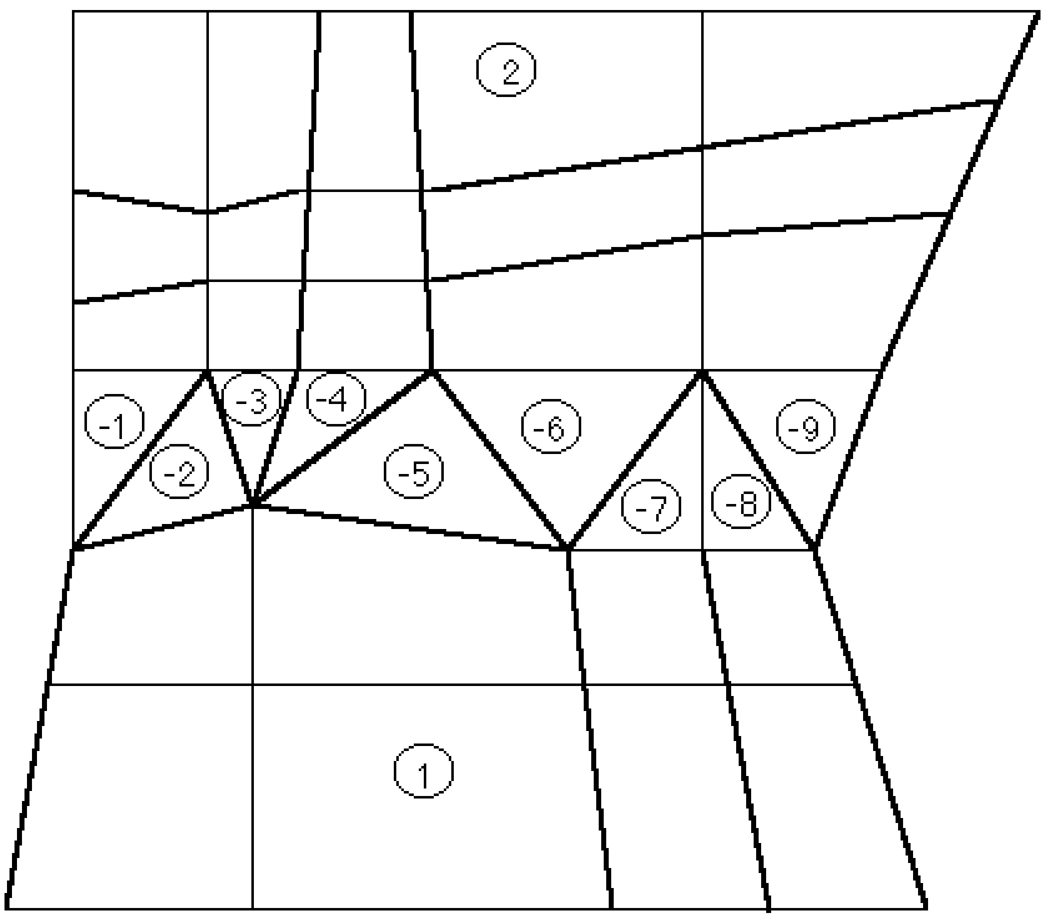


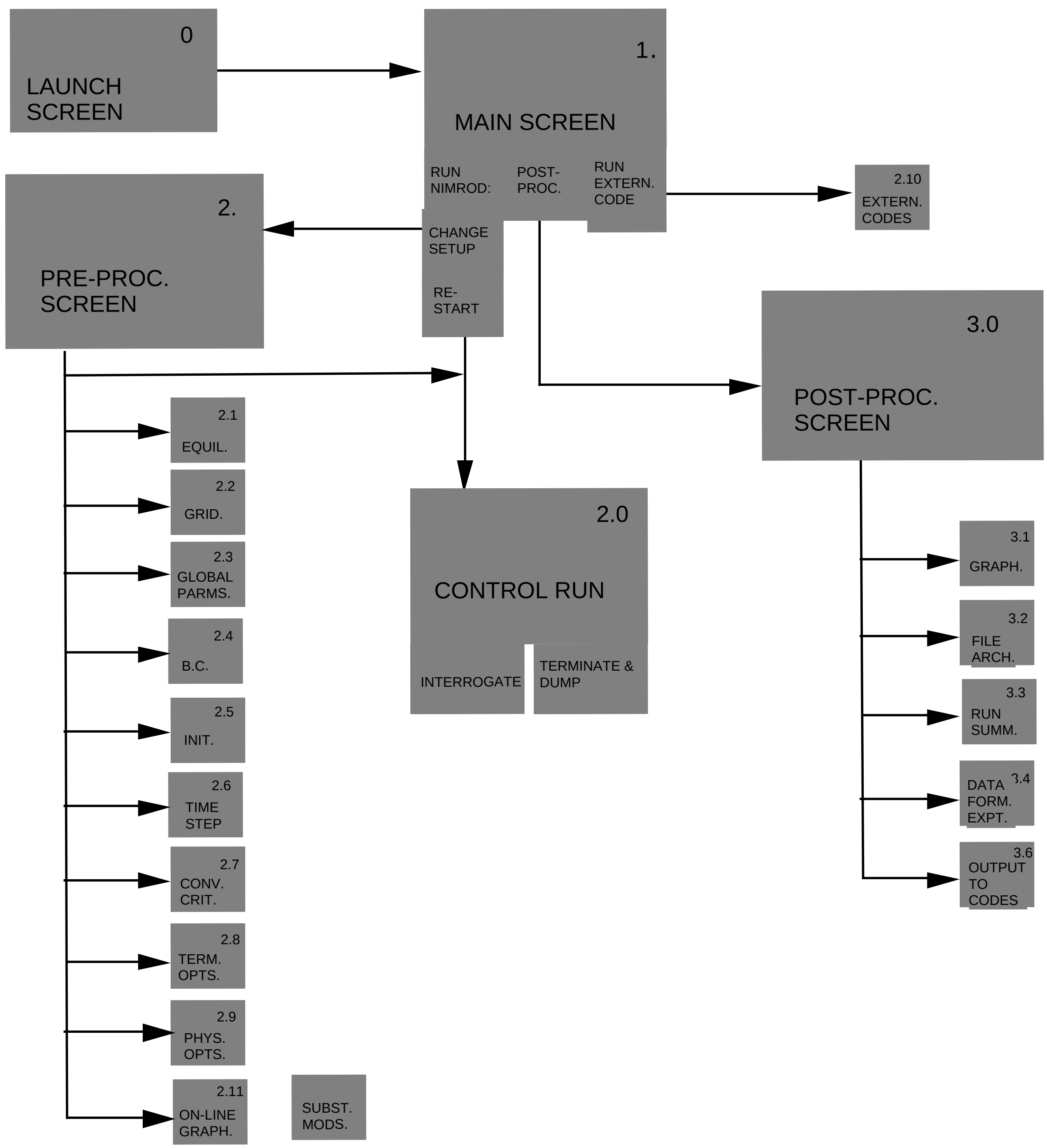
PROGRAMMING STANDARDS

- Fortran90
  - Dynamic memory
  - Rich data structures
  - Object-based programming
- Message-passing parallelism (MPI)
  - Portability to any machine with single-processor F90 compiler
  - Allow irregular, asynchronous communication
- Portable code
  - Cray T3E
  - Cray T3D
  - IBM SP2
  - Workstation clusters
  - Cray C90
  - Serial machines
- Still searching for "standard" file format

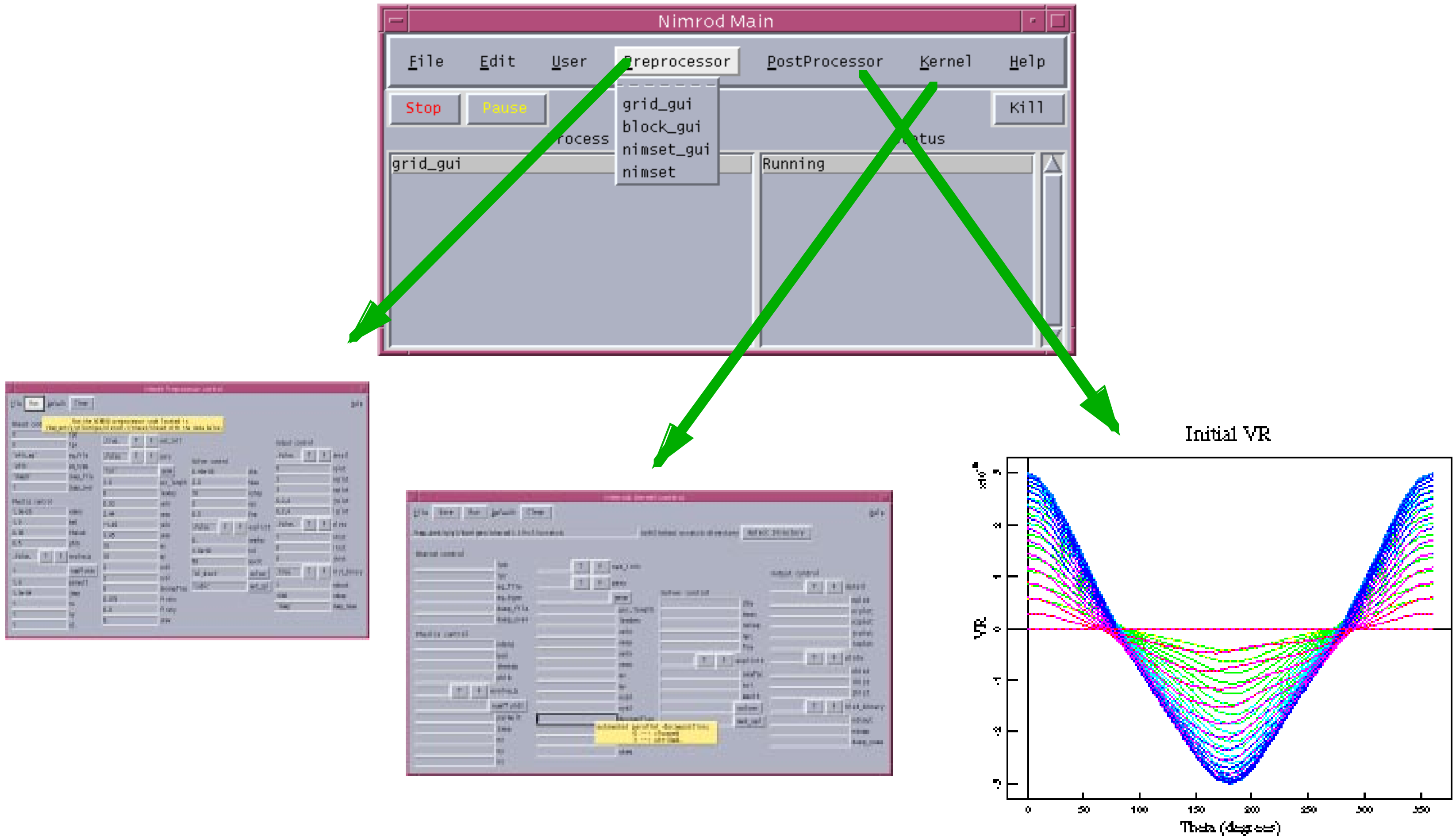
GRAPHICAL USER INTERFACE

- Designed by customers
- Written in tcl/tk
- Controls interaction between user and NIMROD
  - Problem setup
  - Dynamical interaction
  - Run time diagnostics
- Controls interaction between NIMROD and
  - Other user codes
  - Pre-processor
  - Post-processor
  - Graphics/animation
- Commercial software

NIMROD GUI SCREEN FUNCTIONALITY



NIMROD GUI SCREENS



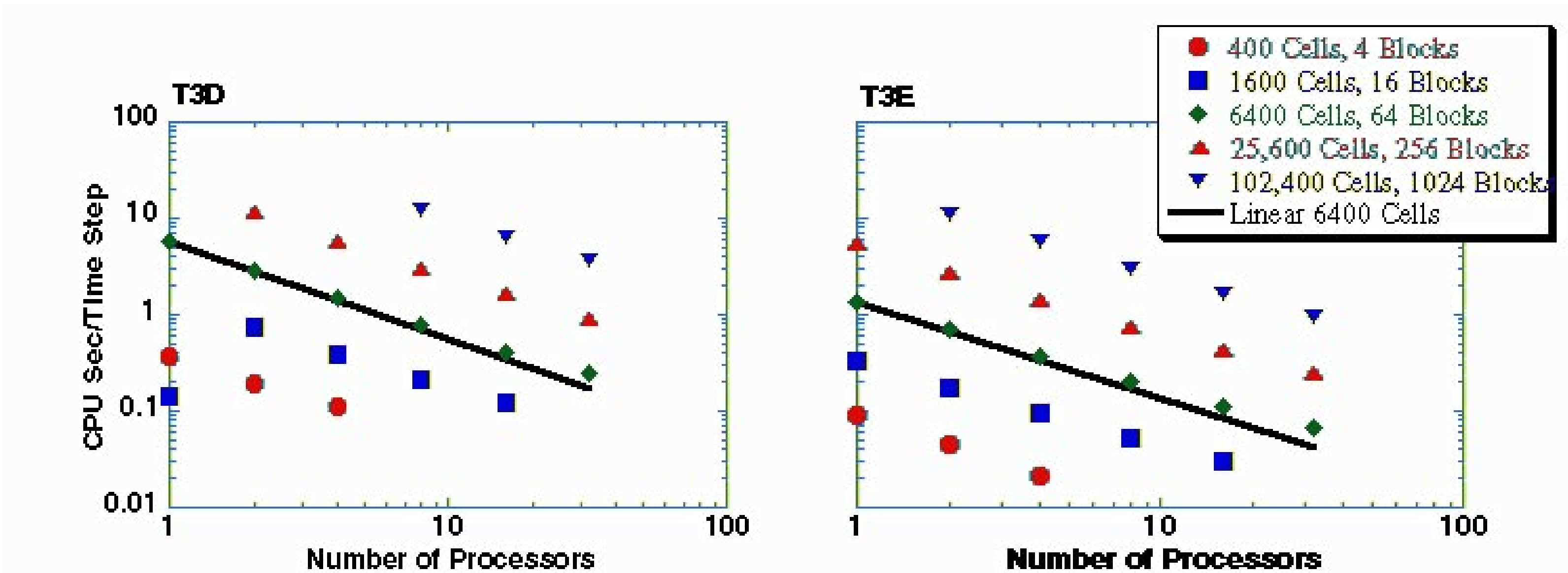
GRAPHICS/ANIMATION

- **Quick-look**
  - **XDRAW**
    - **Time histories**
    - **Contour plots**
  - **Provision for user-defined diagnostics**
- **Detailed analysis**
  - **IBM/DX**
    - **State-of-the-art graphics and animation**
    - **Requires user investment in software and hardware**
  - **Provision for user-defined diagnostics**
- **Interface to other commercial hardware**
  - **HDF files**
    - **Spyglass**
    - **NCSA**
  - **Text files**

PARALLEL COMPUTING

- **MPI**
- **Each processor owns 1 or more blocks**
  - **RBLOCKs**
  - **TBLOCKs**
  - **Computations done on each block independently**
- **Blocks connected by seams**
  - **Data passed between processors**
    - **Explicit calculations**
    - **Matrix-vector multiply in CG solver**
    - **Dot-product in CG solver**
  - **Seam communication a small fraction of block computation time**
- **Preconditioner**
  - **Direct solve within each block**
  - **Patch across seams**

NIMROD PARALLEL PERFORMANCE SCALING AT FIXED PROBLEM SIZE



STATUS

- NIMROD physics kernel
  - Full three-dimensional, nonlinear, cold plasma model implemented
  - Extensive numerical analysis
  - Parallel computations
- GUI
  - Written in tcl/tk
  - Basic functionality
- Pre-processor
  - Interface with EQDISK files
  - Grid generator
  - Input generation
- Post-processor
  - XDRAW generalized to NIMROD grid
  - DX interface written and implemented
- Validation underway

PLANS

- **Warm plasma**
  - Adiabatic energy equations
  - Continuity equations
- **Continue validation**
  - Ideal stable spectrum
  - Ideal internal modes in shaped tokamaks
    - Solovev equilibrium
    - GATO
    - Keldysh ideal MHD codes
    - DCON
  - Resistive modes
    - Keldysh resistive codes
  - ???
- **Continue GUI, pre-processor, post-processor and graphics development**
- **Neo-classical effects, heat conduction, sources, etc.**
- **Time scale:**
  - Beta-test version to GA: Summer 1997
  - First "production" version: Summer 1998