N93-26961

Next Generation System Modeling of NTR Systems

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Los Alamos National Laboratory
October 22, 1992

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Introduction

- NTR Modeling Challenges
- Current Approaches
- Shortcomings of Current Analysis Methods
- Future Needs
- Present Steps Toward These Goals

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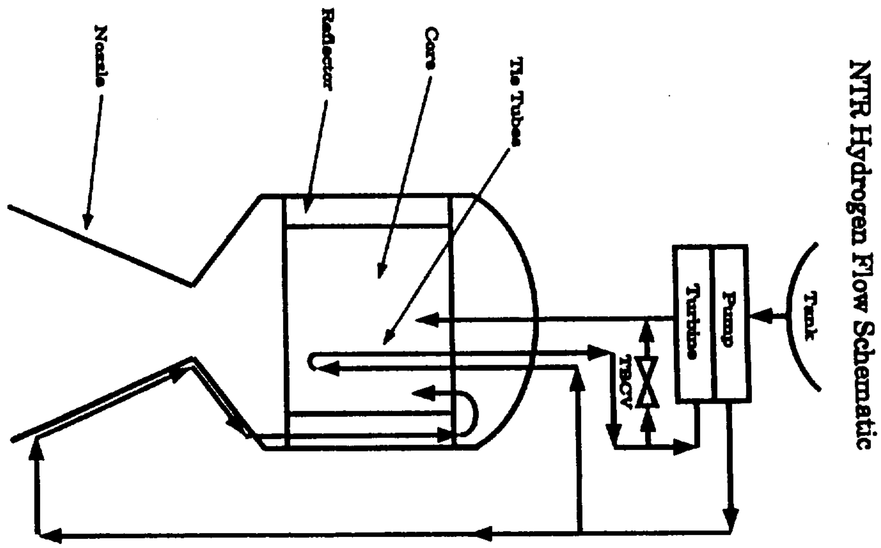

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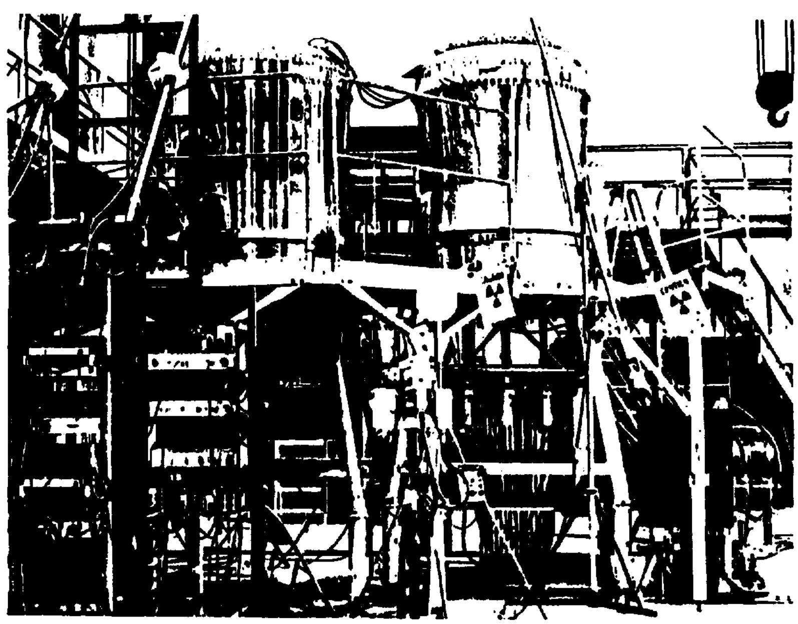
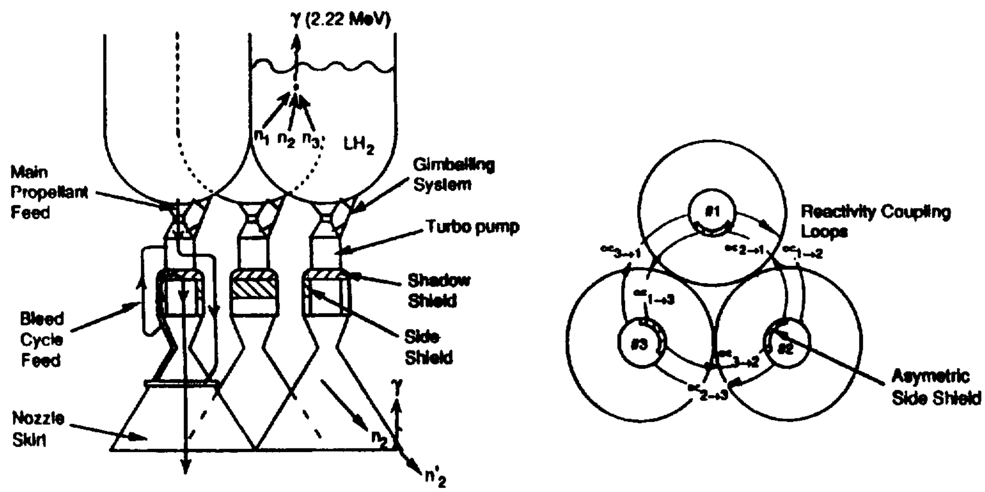


Figure 1. The Coupled Cores in Kiva-3, Pajarito Site. "Test Kiwi" is on the left, and PARKA is on the right.

ENGINE COUPLING PHENOMENA



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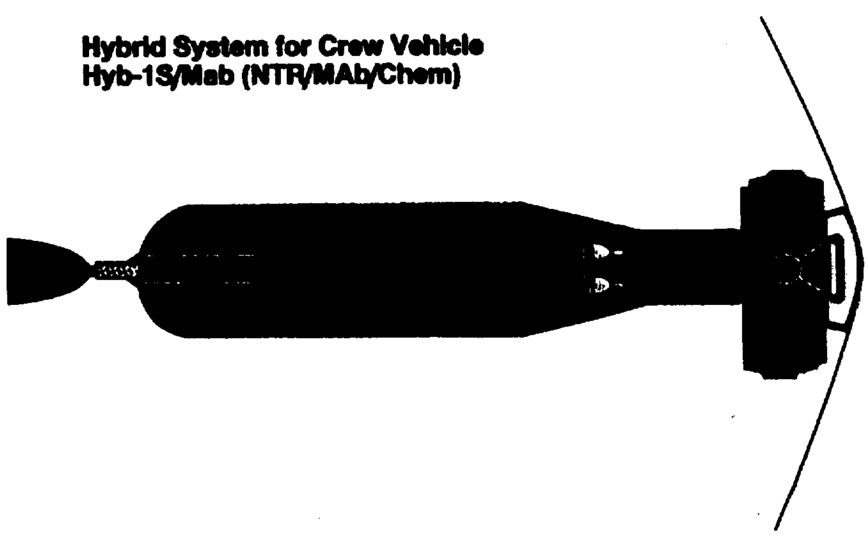

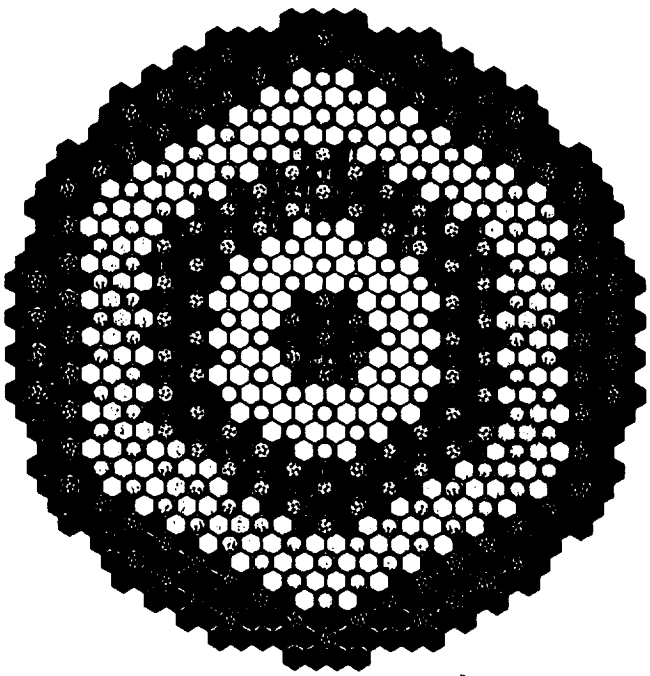

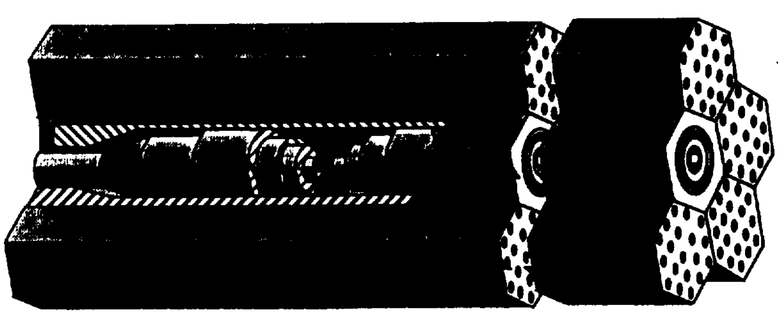

3D NTR Cluster

Introduction: Modeling Applications

- Design: performance (SS operation) and lifetime (fuel / criticality)
- Startup and Shutdown
  (two phase T-H, neutronics, kinetics, heat transfer, low strain rate hydro)
- Water Immersion
  (kinetics, neutronics, all hydro)
- Impaction
  (kinetics, neutronics, high strain rate hydro)
- Engine-Out Operations
  (all except high strain rate hydro)

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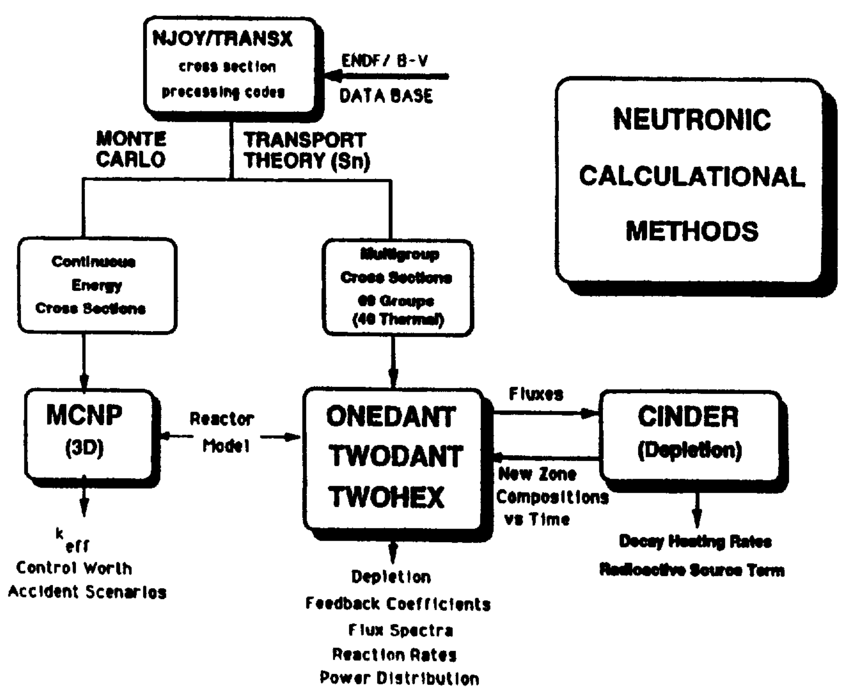

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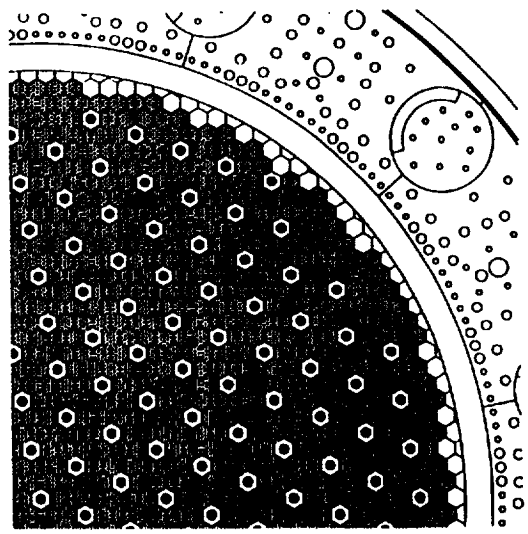
DETAILED MCNP MODELING OF NUCLEAR THERMAL ROCKETS – WESTINGHOUSE NRX-A6 REACTOR



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Thermal-Hydraulic Analysis Methods

- Extensive experience in both space and terrestrial reactors
- **TRAC**
  - Developed for LOCA analysis of PWRs
  - Highly developed models for two-phase flow
  - Low/zero gravity models are available
  - Useful for facility/more general system analysis
- **HERA**
  - Developed for solid core terrestrial reactors
  - Useful for the thermal analysis of general systems including space nuclear systems
- **KLAXON**
  - New thermal hydraulic systems code designed specifically for gas cooled, space reactors
- **THROHPUT**
  - State-of-the-art heat pipe modeling from startup to shutdown

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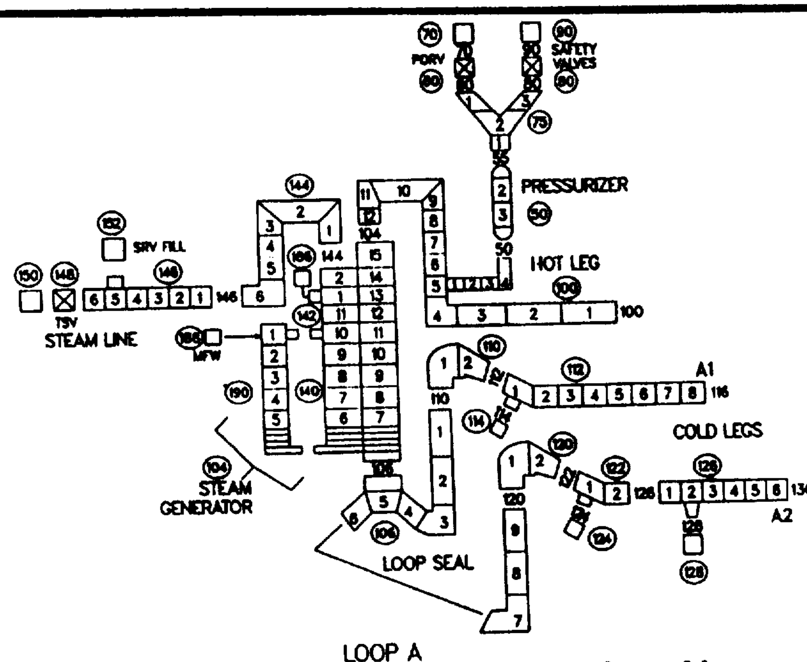
Example TRAC Noding Diagram



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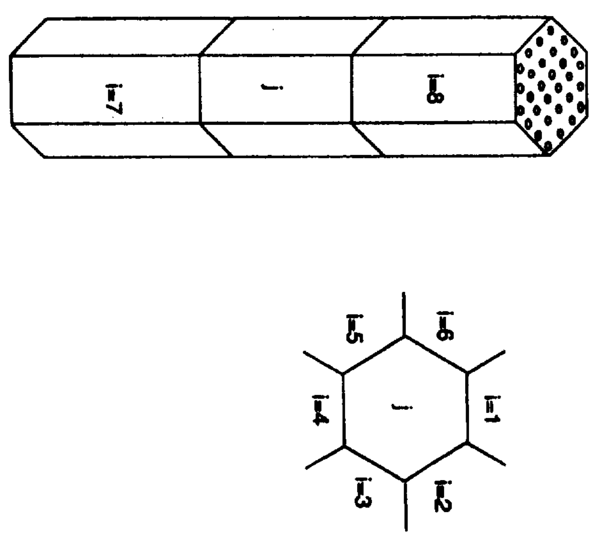
Description of HERA



- HElium Reactor Analysis
- Fully three-dimensional allowing for complex geometries to be accurately represented.
- Flexible input allows a large number of test cases.
- The code computes solution with minimal computational effort.

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Thermal-Hydraulic Modeling: Prismatic Fuel

- HERA: HElium/Hydrogen Reactor Analysis
- Used to model reactor core and core components with axially homogeneous construction
- Three-dimensional, fully transient, arbitrary user defined geometries
- Programmed to be computationally efficient, especially on vector supercomputers
- Currently exists in stand-alone mode and coupled to TRAC. Connection to KLAXON is planned
- PATRAN grid generator and visualization translators currently being written
- Coupling to Storm's corrosion model envisioned → **Core Lifetime**
- Component and core T-H model planned (fuel element, support element, and periphery)

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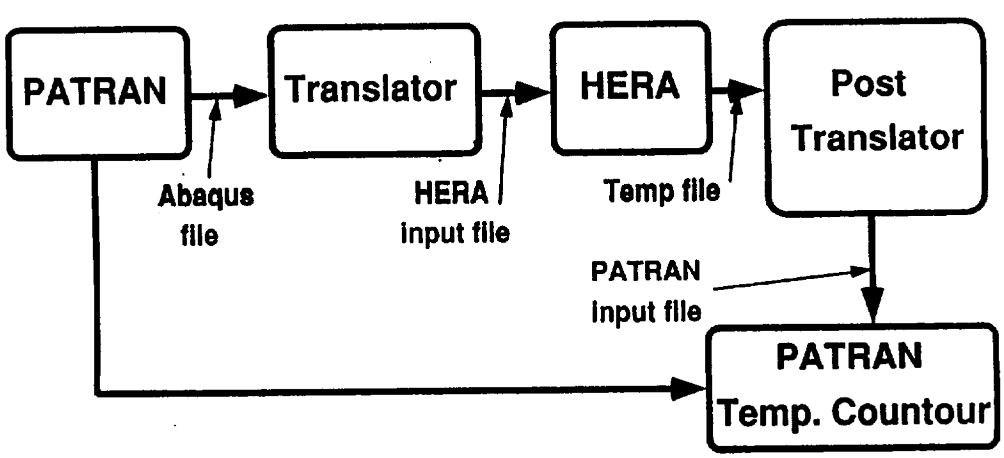
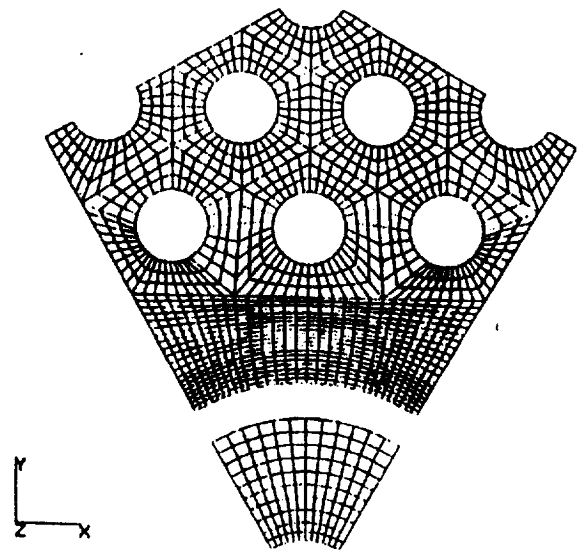
Methodology: New

Specific Outline:

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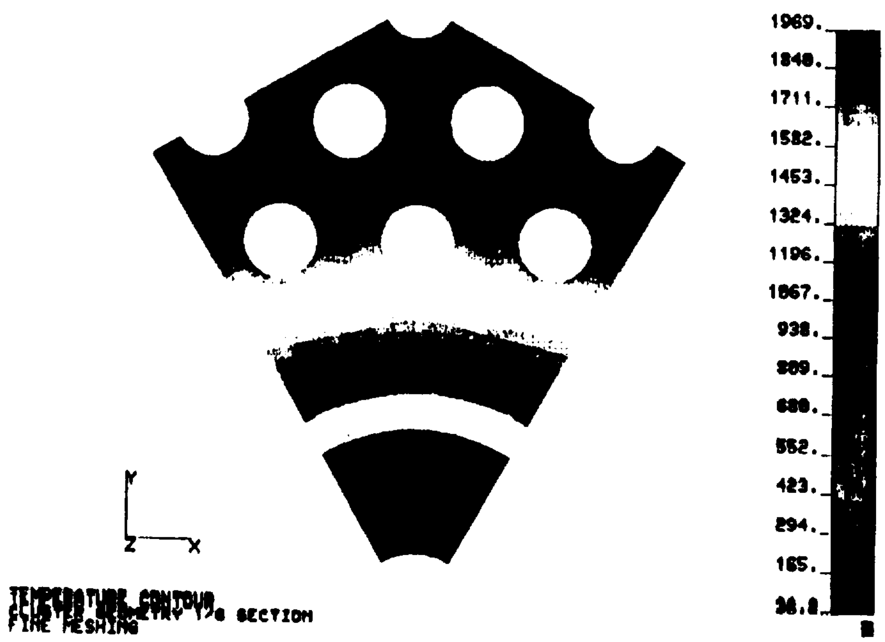
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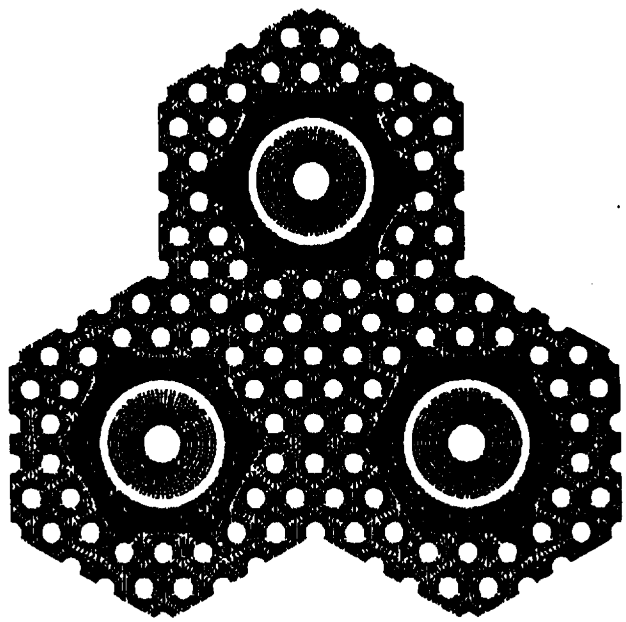
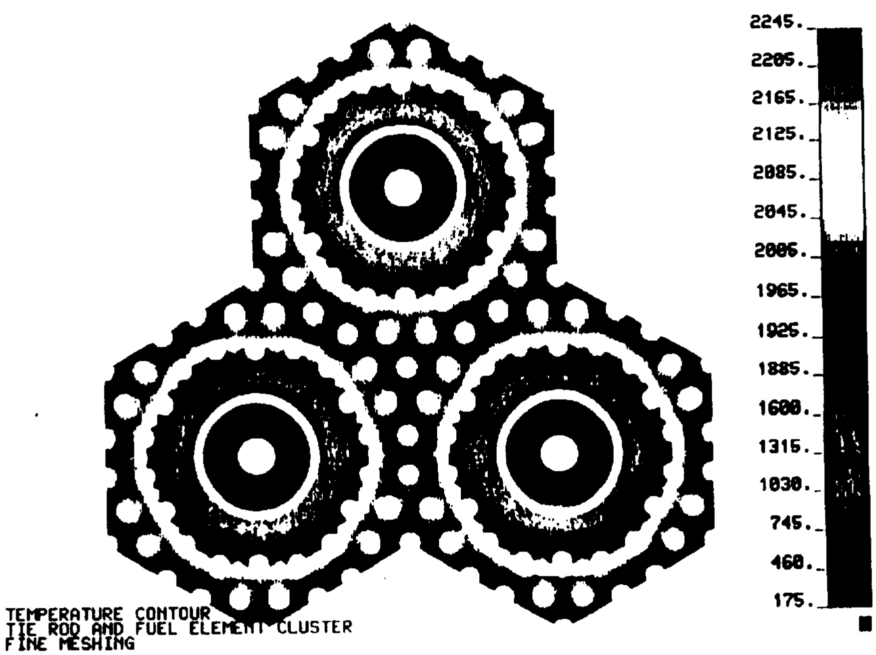
TEMPERATURE CONTOUR
CLUSTER GEOMETRY 1/6 SECTION
FINE MESHING

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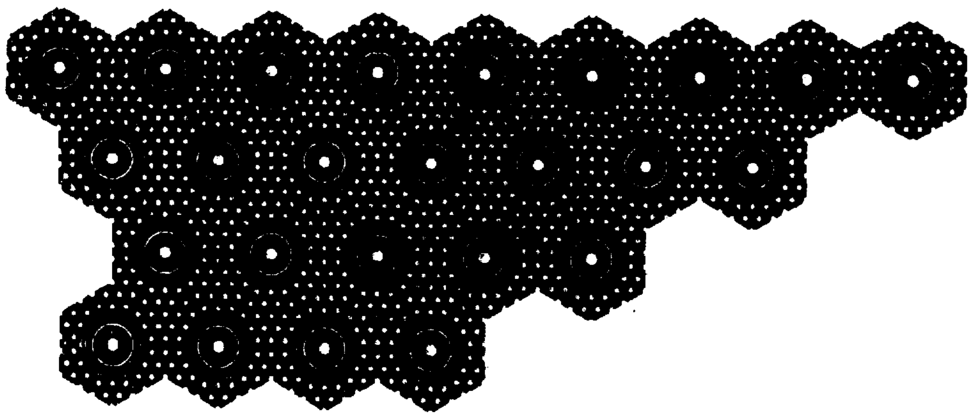
TEMPERATURE CONTOUR
TIE ROD AND FUEL ELEMENT CLUSTER
FINE MESHING

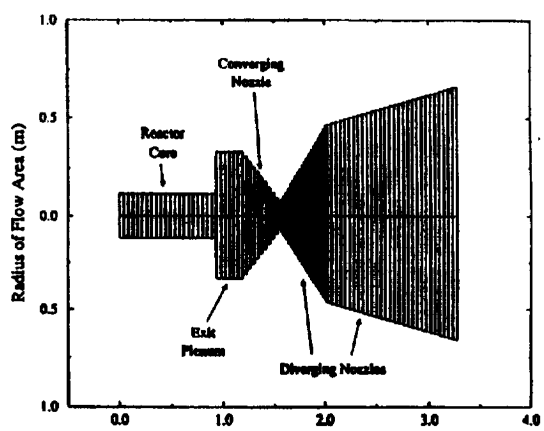


KLAXON
GAS-COOLED REACTOR SYSTEMS MODELING CODE

Time-dependent analysis of systems operating with compressible gas working fluids. TRAC-like pipe, plenum, etc. component models, fill and break capabilities, and advanced flow modeling numerics for shock following in nozzles.

Future Development

- **Connection to HERA**
- **Validation with systems data**



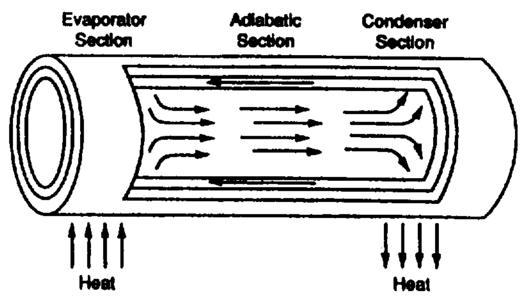
NTR Geometry

THROHPUT
HEAT PIPE MODELING CODE

Transient thermal-hydraulic heat pipe modeling code with:

- **Multi-region capability (wall, fluid, mixed, gas)**
- **2-D convection and conduction heat transfer**
- **Li melt model**
- **Gravity and non-gravity capillary pressure models**

Future development:
Benchmarking and validation with LANL experiments



Heat Pipe Operation

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Why Level 3/4 Model Development?

- Level 3/4 Improvements
  - Integral versus Ad hoc
  - Physics versus Assumptions
  - Confidence versus Safety Margin
  - Machine versus Human Intervention
- Examples
  - Reactor Compaction/Immersion Accidents
  - Reactor Startup

Future Needs

- ❒ Better All Around Resolution of Problems
- ❒ System Design Optimization Tools
- ❒ Complete Utilization of Modern Technology (Computers and Algorithms)
- ❒ Use of Integrated Physics Codes

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REACTOR DESIGN AND ANALYSIS GROUP

Los Alamos Perspective

- **Emphasis on Simulation Instead of Testing**
  - current ES&H environment dictates reduced testing of nuclear systems
- **Interagency NTP Modeling Team**
  - Role, Impact, Importance, Visibility
- **Effort Should be Commensurate With the SEI**
  - ambitious, high profile, high tech, national importance

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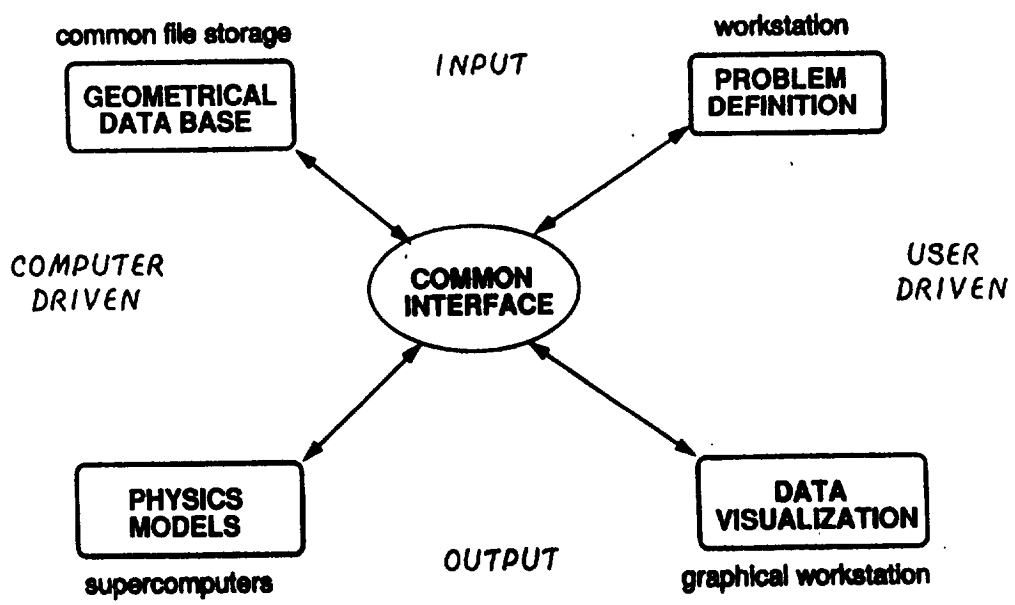
The Need for New Code Development in Level 3/4

- No "Real" Level 3/4 Codes Exist
- Codes will be Heavily Relied on
- Testing will be Restricted by ES&H Requirements
- Current Codes are Designed to Analyze Primarily Terrestrial Reactors
- Current Codes use Outdated Methodologies
- Current Codes are Designed for Older Computer Architectures

2

Advanced Architecture: Description



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Advanced Architecture: Potential Physics Packages

- Neutronics (including cross-sections, dosimetry)
- Spatial Kinetics
- Generation/Depletion
- Thermal-Hydraulics (two phase)
- Low Strain Rate Hydro
- High Strain Rate Hydro (solid and fluid)
- Heat transfer (conduction, radiation)
- Chemistry/Materials

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LANL Current Status

- Outlined Needs and Requirement for Level 3/4 Code Development
- Investigated LANL Capability
- Example LANL Capability
  - NIKE — A time-dependent S_n radiation transport code with arbitrary 3-D meshes on a CM (or Cray)
  - NIKE is coupled to PAGOSA/X3D for high strain rate hydrodynamics on CM (or Cray)
  - Genesis of Level 3/4 code capability for compaction/immersion accident analysis
  - Starting demonstrative NIKE/PAGOSA NTR analysis effort
  - Thermal-hydraulic work continues with work on improving both KLAXON and HERA

3

- Fluid dynamics codes
  - Developed for a large range of physical situations varying from incompressible to highly compressible flows
  - Advanced methodologies
- High Strain Rate Solid/Hydrodynamics
  - Applicable to events involving reactor impaction/disassembly
  - Examples: launch accidents, reentry, water immersion
  - Coupled directly to other physical phenomena (neutronics for instance)
  - Advanced methodologies
- High Performance Computing
  - One of two DOE centers of excellence
  - ICN (3 CMs, 7 Cray YMPs)
  - ACL

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ADVANCED COMPUTING LABORATORY

Acting as a university/industrial/laboratory interface for state of the art computations, emphasizing:

- State of the art hardware for massively parallel computation (largest CM-2s and CM-5 in the nation)
- Wide area gigabit network for distributed parallel computing (using ANSI standard: HIPPI)
- Advanced scientific visualization using high speed networking and parallel computational methods
- Software tools/algorithms development for distributed parallel computation (NSF Science & Tech. center: CRPC)
- Emphasizing "real" applications running in parallel environment (Grand Challenges and beyond)

Purposes of the ACL

- To respond to the rapid changes in hardware and software
- To investigate new "Grand Challenge" computing environments
- To provide more "access" to Los Alamos from the outside world
- Provide high performance testbed for networking and visualization
- Stimulate practical algorithm development for massively parallel computing
- Function as one of the Dept of Energy High Performance Computing Research Centers

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Table 1: TODAY

Project	Description	Operations	Memory	Data Access
Porous Media	2-d immiscible flow	10^{16}	8 Gbytes	40 GBytes
Novel Materials	2-d molecular dynamics	10^{14}	500 Mbytes	64 GBytes
	3-d multimaterial hydro (200^3 pts)	10^{15}	8 GBytes	100GBytes
Plasma physics	transport scaling	10^{15}	8 GBytes	200 GBytes
Global Ocean	decade, 20 levels, 1/2°	10^{15}	500 MBytes	250 GBytes
Brain Topology	3-d reconstruction	10^{13}	200 MBytes	10 GBytes
QCD	quenched lattice (32x32x32x64)	10^{16}	500 MBytes	500 MBytes

Table 1: TOMORROW

[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Porous Media	3-d immiscible flow	10^{18}	1 Tbytes	4 TBytes
Novel Materials	3-d molecular dynamics	10^{18}	20 Gbytes	3 TBytes
	3-d multimaterial hydro (1000^3 pts)	10^{18}	1 TBytes	20TBytes
Plasma physics	numerical Tokamak	10^{18}	1 TBytes	100 TBytes
Global Ocean	century, 40 levels, 1/4°	10^{17}	4 GBytes	20 TBytes
Brain Topology	3-d reconstruction	10^{15}	15 GBytes	1 TBytes
QCD	quenced lattice (64x64x64x128)	10^{18}	8 GBytes	8 TBytes

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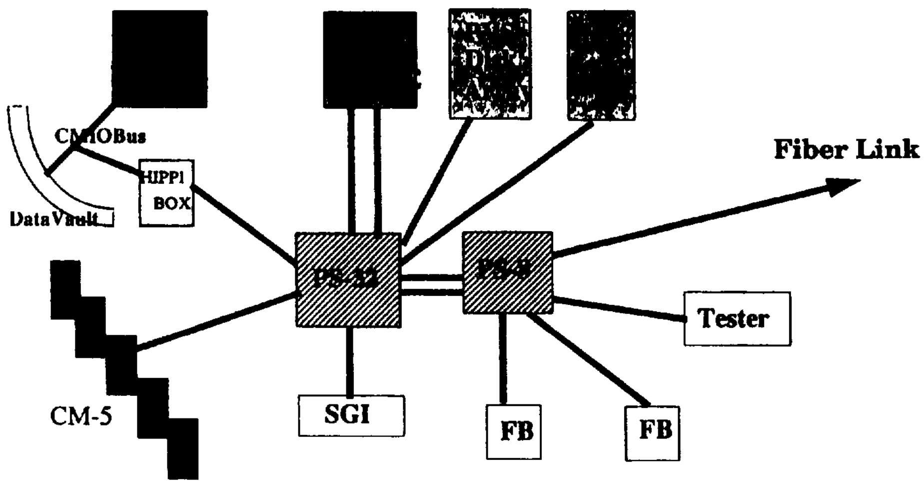
Applications on the CM-2

- QCD
- Condensed Matter Physics
- Free Lagrange Hydrodynamics
- Global Ocean Model
- Lattice Gas (porous media)
- Oil Reservoir: Mobil (11Gflops sustained)
- Tokamak Fluid Turbulence
- Fokker Planck
- Crystal Formation
- Many Body Problem
- Plasma Particle Simulations
- Molecular Dynamics
- Neural Networks

Existing ACL HIPPI Network



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PAGOSA

- A 3-D Multi-Material Hydrodynamics Code on the Connection Machine
- High-Speed Hydrodynamics and High-Rate Deformation of Solids
- Eulerian, Second-Order Predictor Corrector Lagrangian Step with Third-Order High-Resolution Advection
- High-Resolution Interface Reconstruction Algorithm
- Highly Efficient for the Connection Machine

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The NIKE Codes

- NIKE-R
  - 3-D Rectangular Mesh
  - Corner Finite-Difference Scheme
- NIKE-T
  - 3-D Arbitrarily-Connected Tetrahedral Mesh
  - Linear-Continuous Finite-Element Discretization
- Common Characteristics
  - Solve Even-Parity S_n Transport Equation with Anisotropic Scattering in Cartesian Geometry
  - Time-Dependent, Steady-State, k or α Eigenvalue Calculations
  - Essentially Positive Solutions - No Flux Fixup
  - Inner and Outer Iteration DSA - Unconditionally Stable and Effective
  - Very Efficient Simplified P_n Option - No Ray Effects

Conclusions

- ❒ **Current Modeling Approaches are Generally Inadequate**
- ❒ **In the Future Modeling will be Relied on Heavily**
- ❒ Los Alamos **has begun to Lay the Groundwork for Future Modeling Capabilities**

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