Next Generation System
Modeling of NTR Systems

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Los Alamos National Laboratory
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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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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

Hybrid System for Crew Vehicle
Hyb-1S/Mab (NTR/MAb/Chem)
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)
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
Example TRAC Noding Diagram

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Description of HERA

- Hydrogen 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.

NTP: Systems Modeling 718
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
- Component and core T-H model planned (fuel element, support element, and periphery)

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Methodology: New

**Specific Outline:**

```
PATRAN -> Translator -> HERA -> Post Translator
```

Abaque file

HERA input file

Temp file

PATRAN input file

PATRAN

Temp. Countour
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

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NTR Geometry

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NP-TM-92
Transit 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
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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- 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
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

Advanced Architecture: Description

common file storage

user

workstation

INPUT

PROBLEM
DEFINITION

COMPUTER
DRIVEN

COMMON INTERFACE

user

OUTPUT

DATA
VISUALIZATION

graphical workstation

supercomputers

PHYSICS MODELS

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NP-TIM-92 725

NTP: Systems Modeling
### 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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<table>
<thead>
<tr>
<th>LANL Current Status</th>
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<tbody>
<tr>
<td>Outlined Needs and Requirement for Level 3/4</td>
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<tr>
<td>Investigated LANL Capability</td>
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<tr>
<td>Example LANL Capability</td>
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</table>
  - NIKE—a time-dependent, S, radiation transport code with arbitrary 3-D meshes on a CM (or Cray)
  - NIKE is coupled to PACOSA/XSD for high strain rate hydraulic analysis
  - Lessons of Level 3/4 code capability for computation/intension
  - Starting demonstration NIKE/PACOSA NTR analysis effort
  - Thermal-hydraulic work continues with work on improving both KLAON and HERA |

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Other Laboratory Capability

- 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

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

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Table 1: TOMORROW

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</tr>
</tbody>
</table>

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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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Conclusions

Current Modeling Approaches are Generally Inadequate

Los Alamos has begun to Lay the Groundwork for Future Modeling Capabilities

In the Future Modeling will be Relyed on Heavily

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 $\alpha$ Eigenvalue Calculations
  - Essentially Positive Solutions - No Flux Fixup
  - Inner and Outer Iteration DSA - Unconditionally Stable and Effective
  - Very Efficient Simplified $P_3$ Option - No Ray Effects