Status of the Nanoelectronic Modeling tool (NEMO 1-D and 3-D) and its planned extension to Spintronics

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Work performed in collaboration with
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Tim Boykin (U Alabama in Huntsville)

This research was carried out at the Jet Propulsion Laboratory, California Institute of Technology, under a contract with the National Aeronautics and Space Administration
Presentation Outline

- NASA Mission Pull
- Technology Push:
- What is a Quantum Dot?
- Our Project portfolio
  - Modeling / Characterization / Applications
- Quantum Dot Modeling:
  - Tight Binding Parameterization
  - Strain
  - Alloy Disorder
  - Interface Interdiffusion
- NEMO 3-D:
  - Parallelization, Nanotubes, GUI
<table>
<thead>
<tr>
<th>Solar System Exploration</th>
<th>General Technology Requirements</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>near-term</strong></td>
<td></td>
</tr>
<tr>
<td>Pluto (04)</td>
<td>High radiation tolerance</td>
</tr>
<tr>
<td>Europa orbiter (06)</td>
<td>Extreme temperature operation</td>
</tr>
<tr>
<td>Solar Probe (07)</td>
<td>Low weight, low power, high</td>
</tr>
<tr>
<td></td>
<td>performance, high capacity</td>
</tr>
<tr>
<td><strong>long-term</strong></td>
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<tr>
<td>Comet nucleus sample return</td>
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<tr>
<td>Europa lander</td>
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<tr>
<td>Titan explorer</td>
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<tr>
<td><strong>Structure and Evolution of the Universe (SEU)</strong></td>
<td></td>
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<tr>
<td>14 projects</td>
<td><strong>Defined IT Requirements</strong></td>
</tr>
<tr>
<td><strong>Sun Earth Connection (SEC)</strong></td>
<td></td>
</tr>
<tr>
<td>10 projects</td>
<td>Closed loop autonomous Guidance Navigation and Control</td>
</tr>
</tbody>
</table>

*NASA missions require systems that currently do not exist*
Planetary Extreme Environments

Radiation total dose, Mrad

Sun Spot

Earth

Comets

Moon

Europa

Ganymede

Mercury

Venus

Io

Temperature, °C

-300 -250 -200 -150 -100 -50 50 100 150 200 250 300 350 400 450 500
Low weight, low power and high efficiency

Have a special meaning to NASA
Commercial market pushes computing performance (FLOPS/weight/power):

- Enabled by device miniaturization
- Enabled by chip size increase
- Limited by: Costs of fabrication
- Limited by: Discrete atoms/electrons

Additional NASA Requirements:

- High radiation tolerance
- Extreme temperature operation-hot/cold
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Quantum Dots Push beyond SIA with near and long term applications
- Detectors / lasers
- Memory and logic

Quantum dots go beyond the SIA roadmap and enable near and long term NASA applications
What is a Quantum Dot?
Basic Application Mechanisms

Physical Structure:
• Well conducting domain surrounded in all 3 dim. by low conducting region(s)
• Domain size on the nanometer scale

Electronic structure:
• Contains a countable number of electrons
• Electron energy may be quantized -> artificial atoms (coupled QD->molecule)
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- Diagram showing processes:
  - Photon Absorption
  - Photon Emission
  - Tunneling/Transport Occupancy of states
  - Detectors/Input
  - Lasers/Output
  - Logic / Memory
What is a Quantum Dot?
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Quantum dots are artificial atoms that can be custom designed for a variety of applications
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Pyramidal or dome shaped</td>
<td></td>
</tr>
<tr>
<td>R.Leon, JPL (1998)</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Nanocrystals:</th>
<th>Molecular Dots</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si implanted in SiO₂</td>
<td>Ruthenium-based molecule</td>
</tr>
<tr>
<td>Atwater, Caltech (1996)</td>
<td>Ru₄(NH₃)₁₆(C₄H₄N₂)₄₁₀⁺</td>
</tr>
<tr>
<td></td>
<td>proposed by Marya Lieberman, Notre Dame</td>
</tr>
<tr>
<td></td>
<td>(1999)</td>
</tr>
</tbody>
</table>

Low Dimensional quantum confinement can be achieved in a variety of material systems
Nanotechnology Project Portfolio

- **Modeling**
  - Enable the exploration of the nanotechnology design space.

- **Characterization**
  - Optical, structural, transport and radiation testing.

- **Devices**
  - **Lasers / Output:**
    Enable radiation hard, narrow linewidth tunable lasers.
  - **Sensors / Input:**
    Enable acoustic and electronic sensors based on nanotubes.
  - **Memory:**
    Enable high density, low power, non-volatile, radiation hard storage.

- **Architectures:**
  - Enable massively parallel and fault tolerant computing architectures.

*Future deep space applications will directly benefit from directed nanotechnology research*
**Quantum Dot Modeling - Development of Bottom-Up Nanoelectronic Modeling Tool**

**Nano-scale Device Analysis / Synthesis**

**Development of a Bottom-Up Nanoelectronic Modeling Tool**

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### Assertions / Problems:
- Nanoscale electronic structures are built today! The design space is huge: choice of materials, compositions, doping, size, shape.
- Radiation on today’s sub-micron devices modifies the electronics on a nanoscale.

### Approach:
- Deliver a 3-D atomistic simulation tool
- Enable analysis of arbitrary crystal structures, particles, atom compositions and bond/structure at arbitrary temperatures and ambient electric and magnetic fields.

### Collaborators:
- U. of Alabama, Ames, Purdue

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### NASA Relevance:
- Enable new devices needed for NASA missions beyond existing industry roadmap:
  - Water detection -> 2-5μm Lasers and detectors.
  - Avionics -> High density, low power computing.
- Analyze state-of-the-art devices for non-commercial environments:
  - Europa -> Radiation and low temperature effects. Aging and failure modes.
  - Jovian system -> Magnetic field effects
  - Venus -> high temperature materials: SiGe

### Impact:
- Low cost development of revolutionary technology
- Narrow empirical/experimental search space

---

*Modeling will narrow the empirical search space!*
Need for Nanoelectronic Simulation

Problems:
- Design space is huge
  - Choice of materials, shapes, orientations, dopings, heat anneals
- Characterizations are incomplete and invasive / destructive

Simulation Impact:
- Aide Design
  - Fast, cost effective.
  - Device performance already successful for 1-D quantum devices
- Aide Characterization
  - Non-invasive
  - More accurate
  - Structure and doping analysis already successful for 1-D quantum devices

Modeling, Characterization and Fabrication are inseparable for nanoscale devices
Objective

- **Long term objective:**
  - Develop and demonstrate a physics-based, atomistic simulation tool for semiconductor quantum dots and molecular based electronic devices

- **Near term objective:**
  - Develop this year the technology necessary to simulate optical transitions in a single quantum dot

- **Tasks in FY 00:**
  - Alloysed dot simulation (04/00)
  - Shared memory parallelization (05/00)
  - 3-D visualization (05/00)
  - Atomistic grading simulation (07/00)
  - Atomistic impurity simulation (09/00)

*We build a bottom-up, atomistic nanoelectronic design tool*
### Related Work

<table>
<thead>
<tr>
<th>Investigator</th>
<th>Location</th>
<th>Hamiltonian</th>
<th>Atomistic</th>
<th>Many-Body</th>
<th>Extendable to Molecules?</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pryor</td>
<td>Lund</td>
<td>k•p</td>
<td>NO</td>
<td>YES</td>
<td>NO</td>
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<tr>
<td>Bimberg</td>
<td>Berlin</td>
<td>k•p</td>
<td>NO</td>
<td>NO</td>
<td>NO</td>
</tr>
<tr>
<td>Freund</td>
<td>Brown</td>
<td>k•p</td>
<td>NO</td>
<td>NO</td>
<td>NO</td>
</tr>
<tr>
<td>Leburton</td>
<td>Illinois</td>
<td>1 Band</td>
<td>NO</td>
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<tr>
<td>Zunger</td>
<td>NREL</td>
<td>Pseudopotential</td>
<td>YES</td>
<td>NO</td>
<td>NO</td>
</tr>
<tr>
<td>Bowen/Klimeck</td>
<td>JPL</td>
<td>Tight-binding</td>
<td>YES</td>
<td>NO*</td>
<td>YES</td>
</tr>
</tbody>
</table>

* - Planned for 01

Why JPL? JPL has expertise and infrastructure to tackle such large problems.

*We are in an excellent position to simulate molecular electronics from the bottom-up*
Technical Accomplishments (Physics)

- Genetic algorithm based material parameter analysis
  - Establish a material basis set needed for atomistic simulations
- Mechanical strain calculation
  - Enable proper modeling of optical bandgaps
    -> proper tuning of optical transitions
- Alloyed Dot simulation
  - Enable simulation of realistic quantum dot compositions
  - Enable analysis of inhomogeneous linewidth broadening due to alloy disorder
- Atomistic grading simulation
  - Enable simulation of realistic quantum dot interfaces
  - Enable simulation of interface interdiffusion and the resulting modification of the confined quantum states.

We are just starting to explore the capabilities of this simulator!
Technical Accomplishments (Software)

- Parallelization
  - Evaluate performance of 2 different parallel computing paradigms:
    - shared memory (all CPUs can access the same memory)
    - distributed memory (message passing between CPUs)
  => performed a 2 million atom simulation in the distributed model

- Analysis of general molecular inputs -> Nanotubes
  - Enable electronic simulation of “arbitrary” crystal structures generated from other structural simulators.
  => Expansion to Moletronics

- Graphical User Interface Prototype
  - Enable device, material and computer specific input to and output from a supercomputer based simulator.

- 3D Data Visualization
  - Enable visualization of simulation results

3 person years of software work at JPL and 22 person years NEMO leverage enabled the simulation capabilities.
Quantum Dot Modeling - Development of Bottom-Up Nanoelectronic Modeling Tool

Technical Approach

Problem:
Nanoscale device simulation requirements:
- Cannot use bulk / jellium descriptions, need description of the material atom by atom
  => use pseudo-potential or local orbitals
- Consider finite extend, not infinitely periodic
  => local orbital approach
- Need to include about one million atoms.
  => need massively parallel computers
- The design space is huge: choice of materials, compositions, doping, size, shape.
  => need a design tool

Approach:
- Use local orbital description for individual atoms in arbitrary crystal / bonding configuration
  - Use s, p, and d orbitals depending on the material.
  - Use genetic algorithm to determine material parameter fitting
- Compute mechanical strain in the system.
- Develop efficient parallel algorithms to generate eigenvalues/vectors of very large matrices (N=40 million for a 2 million atom system).
- Develop prototype for a graphical user interface based nanoelectronic modeling tool (NEMO-3D)

Realistic material description at the atomic level enables simulation of realistic nanoelectronic devices.
Genetic algorithm based material parameter analysis

Problem:
- Want atomistic / orbital based material description.
- Need to fit 15-30 orbital interaction energies to 20-30 material properties (bandgaps and masses)

Approach:
- Use massively parallel genetic algorithm to perform multidimensional optimization

Results/Impact:
- Established a 3x3 array of materials and their parameters that are the building blocks of quantum dots.
- Enable the atomistic simulation of quantum dots.

Genetic algorithm enabled the establishment of a material basis set.
**Problem:**
- Self-assembly dot formation due to strain
- Small mechanical strain (5% bond length) -> dramatic effects on electronic structures

**Approach:**
- Nanomechanical strain calculation
- Nanoelectronic strain calculation.

**Mechanics Problem:** Minimize elastic strain (Keating)

**Results:**
- Implemented a mechanical strain model.
- Implemented atomistic bandstructure model that comprehends strain.

**Impact:**
- Can simulate realistic quantum dots.
- Can estimate optical transition energies properly.

**Electronics Problem:** Effect of overlap changes

Orbital overlap changes
=> bandgaps and masses

Pyramidal InAs Dot Simulation
Base: 7nmx7nm  Height: 3nm  Embedded in GaAs

Small strain has dramatic effects on the electronic structure.
# Alloy Disorder in Quantum Dots

**Problem:**
- Cations are randomly distributed in alloy dots.
- Does alloy disorder limit electronic structure uniformity for dot ensembles?

**Approach:**
- Simulate a statistical ensemble of alloyed dots.
- Requires atomistic simulation tool.

<table>
<thead>
<tr>
<th><strong>Results:</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>- Simulated 50 dots with random cation distributions.</td>
</tr>
<tr>
<td>- Inhomogeneous broadening factor of 9.4 meV due to alloy disorder.</td>
</tr>
</tbody>
</table>

**Impact:**
- Fundamental uniformity limit for ensemble of alloy-based quantum dots.

---

**In**

In$_{0.6}$Ga$_{0.4}$As Lense Shaped Dot

(Diameter=30nm, Height=5nm, GaAs embedded)

In and Ga atoms are randomly distributed

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**Simulation of Alloy Dot Ensemble**

\[ \Gamma = 9.4 \text{ meV} \]

\[ E_{eh} = 1.05 \text{ eV} \]

---

**Alloy disorder presents a theoretical lower limit on optical linewidths**
Atomistic Grading Simulation

Problem:
- Quantum dot interfaces may not be sharp.
- There may be cation redistribution around the interface => grading of the concentration.
- How does the interfacial grading affect the electronic structure?

Approach:
- Simulate quantum dot atomistically with graded interfaces as a function of interdiffusion length.

Results:
- More Ga in the quantum dot raises the energy of the transition energies.
- Less Ga in the barriers softens the barriers, reduces the binding of the excited states to the quantum dot and reduces $\Delta E = E_2 - E_1$.

Impact:
- Verify experimentally suggested interdiffusion process may be responsible for blue shift and reduction in $\Delta E$.

Cartoon Visualization of Interdiffusion

Slice through 2 Qdots with thickness of 3 atoms - with and without interdiffusion.

- Ga
- In
- As

Pyramidal InAs in GaAs, Diameter=10nm, Height=4.2nm 5 samples per data point

Interdiffusion widens the bandgap => blueshift
Code Parallelization

Problem:
- Need to calculate eigenvalues of a complex matrix of the order of 40 million.
  => must parallelize code

Approach:
- Evaluate 2 parallel programming paradigms
  - Shared memory (OpenMP) - CPUs can access the same memory.
  - Distributed memory - CPUs exchange data through messages (MPI) - data synchronization performed explicitly by program.

Vision:
- Utilize a designated beowulf cluster of PC’s as a workhorse for these simulations. Each node might have 1-4 shared memory CPUs on one motherboard.
- Envision a “mixed” code with outer level MPI parallelism and inner level OpenMP parallelism.
  - This will run on a commercial supercomputer like an SGI Origin 2000 as well as a beowulf.

Results:
- Inner level OpenMP parallelism does not speed up code significantly. Dynamic creation and destruction of threads is too expensive.
- Decided to abandon the OpenMP implementation and concentrate on the optimization and scaling of the MPI version.

Impact:
- Enabled simulation of 2 million atom systems with 20 orbitals on each atom
  => matrix of order 40million

Cluster of commodity PC’s can beat a supercomputer for our problem
Quantum Dot Modeling - Development of Bottom-Up Nanoelectronic Modeling Tool

Incorporate Arbitrary Molecular Files -> Nanotubes

Background:
- Carbon Nanotubes are currently explored for electronic and structural applications.

Objective/Motivation:
- Simulate optical interactions and electron transport in nanotubes

Problem:
- Need nanotube structural information.
- We do not have that expertise.

Approach:
- Expanded code to read standard chemical structure file format.
- Get structural information from other researchers.

Result:
- Simulated nanotube ground states and density of states.

Possible Cooperation from Nanospace 2000 Conference:
- Optical Characterization Rice
- Structural Simulation Ames, Bonn
- Electronic/Optical Simulation JPL

Preliminary Data

Finite size nanotube ground and excited state

Density of States

We can input molecular dynamics based files and perform electronic structure calculations
Quantum Dot Modeling - Development of Bottom-Up Nanoelectronic Modeling Tool

Software Structure Prototype/Vision

Objective:
- Design, develop, test and deliver an interactive quantum dev. design tool
- Customers: Experimentalists not Simulation Specialists!

Problem:
- Simulations are CPU intensive
  -> need supercomputers
- Datasets are typically 4-dim
  -> need custom visualization
- Local workstations are PC, MAC, SUN or SGI
  -> need portable Graph. User Interf.
- Input requirements change fast
  -> need dynamic GUI design

Approach:
- Heterogeneous client-server Tcl/Tk-based GUI

Impact:
- Using this approach on 2 completely independent simulators with little additional development time.

Flexible software design enables use in various different simulators.
Have built most of the essential components, need to go through integration process.
Quantum Dot Modeling - Development of Bottom-Up Nanoelectronic Modeling Tool

Plans

Plans for FY 01:

- Simulation of ensembles of alloyed quantum dots
  - Study fundamental limit of spectral lines due to alloy disorder
- Simulation of many-body effects via configuration interaction
  - Simulate optical transitions including effects of excitons
- Electron transport through quantum dot
  - Explore design possibilities for electronic transport devices

Plans for FY 02:

- Transport through Nanotubes, DNA including bond deformation effects

Plans for outgoing years:

- Develop a world-class 3-d nanoelectronic modeling tool
Conclusions / Future Vision

- Parallelization (2 million atoms), visualization
- Graded junctions, alloy disorder, strain

- Made significant progress towards a general atomistic simulation tool
- Envision this tool to have impact on quantum dots, end of SIA roadmap issues, and molelectronics.

---

Quantum Dots
Grading

Atomistic Simulation
Graded Abrupt

Transport in Molecules
Carbon Nanotubes
DNA

End of SIA Roadmap
Dopant Fluctuations in Ultra-scaled CMOS
Electron Transport in Exotic Dielectrics

(Ba,Sr)TiO₃
TiO₂

The best is still to come!
Backup Foils
Objectives:

COMPUTERS
- Quantum Dots can enable new types of computing architectures (for example QCA).

MEMORIES
- QDs can be used in ultra-high density optical memories.

RADIATION TOLERANCE
- QDs enable radiation-hard opto-electronic devices.

Approach:

- Achieve positional order of Quantum Dots (QDs) by combining patterning and various types of growth experiments.
- Implement experimental capabilities for in-house QD characterization.
- Collaborate with Universities on fabrication, growth experiments, and characterization.
- Perform tests and experiments on existing QD structures - understand QD properties and how they impact their various device applications.
Objective:
- Design and fabricate high efficient, low power consumption, radiation hard QD based optoelectronic devices, such as:
  - lasers
    - ultralow threshold current density
    - temperature insensitive
    - narrow linewidth

NASA applications:
- Large format, low noise IR detector arrays are enabling technology for SSE
- Broad area of applicability:
  - Spectroscopy
  - Microinstruments
  - Communications
  - LIDAR and Interferometry

Collaborators:
- University of New Mexico
Task Purpose/Objectives:

- Develop a *room-temperature, radiation-tolerant* memory technology based on single-electron storage.
- Decrease read/write time by orders of magnitude using a novel peaked-tunnel-barrier concept.
- Increase capability for computing storage by increasing storage density and decreasing storage power.

Major Products:

- Silicon nanocrystal floating-gate memory
- Shape-engineered tunnel barrier for breakthrough read/write speed.

NASA Relevance:

- **Space Science**: (autonomous spacecraft systems and robots)
- **Earth Science**: (autonomous navigation / guidance; sensing and sensor webs)
- **Human Exploration**: (autonomous robotic monitoring systems)
Objective:

- Develop new logic gates and circuits with emphasis on fault tolerance capabilities.
- Develop massively parallel computing architectures by exploiting inherent features of QCA.

Accomplishments:

- Alternative design of highly fault tolerant logic gates based on arrays of QCA.
- Massively parallel computing architectures for a set of signal/image processing applications.

NASA Relevance:

- Enable smaller and smarter spacecraft by providing drastic improvement over VLSI technology in terms of
  - Integration density
  - Mass, volume, and power consumption
  - Radiation tolerance
  - Enabling novel applications

External Collaborators:

- University of Notre Dame
- Oak Ridge National Laboratory

QCA: A totally new computing paradigm

Challenges: Architecture and Application Design, Fault Tolerance
## Motivation / Impact:
- Nanotubes combine useful properties and nanoscale dimensions
- NT-based electro-mechanical devices provide enabling technology for NASA missions: e.g., biomolecular probes, nanoexplorers

## Objective:
- **Demonstrate prototype nanotube-based devices**
  - NT electrophoresis system
  - Biomimetic acoustic sensor
  - NT actuators
  - NT high-Q resonators
  - NT electronic components

## NASA Applications:
- Search for life via acoustic and molecular signatures
- Nanoscale fabrication and characterization
- Revolutionary computing components
- Intense electron sources
Motivation / Customers

• NASA Relevance:
  – Enable devices needed for NASA missions beyond existing industry roadmap:
    • 2-5µm lasers and detectors
    • High density, low power computation (logic and memory)
    • Life signature biosensors

• Impact:
  – Low cost development of revolutionary technology.
  – Narrow empirical/experimental search space

• Customers / Missions:
  – CISM
  – MDL
  – HPCC
Potential Benefits / Payoffs

NASA Relevance:
- 2-5mm Lasers and detectors
- High density, low power computation (logic and memory)
- Life signature biosensors

Impact:
- Narrow empirical/experimental search space
- Low cost development of revolutionary technology.
Delivery of a Simulation Tool
Quantum Dot Modeling - Development of Bottom-Up Nanoelectronic Modeling Tool

Batch Dataflow is Linear
GUI Data Flow is Continuous

GUI interacts with different software blocks continuously
### Quantum Dot Modeling - Development of Bottom-Up Nanoelectronic Modeling Tool

**Hierarchial Ordering of User Input**

<table>
<thead>
<tr>
<th>Semi-class. self-cons. pot. &amp; single band current</th>
<th>Quantum self-cons. potential &amp; single band current</th>
</tr>
</thead>
<tbody>
<tr>
<td>Specify desired outputs</td>
<td>exchange &amp; correlation?</td>
</tr>
<tr>
<td>Quantum region: “Where are wave-functions?”</td>
<td>how to go from bias to bias?</td>
</tr>
<tr>
<td>Non-equilibrium region: “Where are the reservoirs?”</td>
<td>Specify desired outputs</td>
</tr>
<tr>
<td>Adaptive energy grid</td>
<td>Quantum region: “Where are wave-functions?”</td>
</tr>
<tr>
<td></td>
<td>Non-equilibrium region: “Where are the reservoirs?”</td>
</tr>
<tr>
<td></td>
<td>Quantum Charge region: “Where is the charge quantum mechanically calculated?”</td>
</tr>
<tr>
<td></td>
<td>Resonances-based energy grid</td>
</tr>
</tbody>
</table>

Ask user for input that is really needed.

-> User input determines the sequence of simulation parameter windows.
Dynamic GUI Design.
- data structure
- member descriptor
-> I/O for GUI or files

Data Structure
PotType potential
real hbarovertau
Boolean Ec
RangeStruct NonEq

Translator
Create Read

Graphical User Interface

File/Batch User Interface
potential=Hartree
hbarovertau=0.0066
Ec=FALSE
< start=45, end=69 >