Multi-Physics and Numerical Complexities of Nuclear Reactor Simulation

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Reactor Analysis Group

of the

Nuclear Science and Technology Division

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Outline

- **Background on HOW reactor simulation is done**
- **Discussion of some APPROXIMATIONS used**
- **Examples and their EFFECT on the solutions**
  - **Discussion of WHY solutions are accurate anyways**
- **Conclusions on the need for IMPROVEMENT**

- **But first a word from our sponsors…**

Nuclear @ ORNL

- Nuclear Science & Technology Division (NSTD)
  - Nuclear fuel cycle, medicine, and power (Gen-I through IV and space)
- Global Nuclear Security Technology Division (GNSTD)
  - Nonproliferation, safeguards, threat reduction, and transportation
- Fusion Engineering Division (FED)
  - Teamed with Princeton as the US lead for ITER
- Material Science and Technology Division (MSTD)
  - Radiation effects and chemistry for fuels and structures
- Spallation Neutron Source (SNS)
  - Neutron and atomic physics
- Research Reactor Division (RRD)
  - Materials testing, irradiation research, and isotope production
  - HFIR: High-Flux Isotope Reactor - 80 MWt with HEU plate fuel
- Radiation biology, medical physics, astrophysics, etc.

NUCLEAR SECURITY TECHNOLOGIES

- Material protection, control, and accounting
- Safeguards
- Arms control assessments
- Export control
- Nuclear threat reduction
- Radiation detection
- Radiation transport
- Transportation technologies
- Fissile material detection
- Fissile material disposition
- Instrumentation

NUCLEAR SYSTEMS ANALYSIS, DESIGN, AND SAFETY

- Nuclear data and codes
- Criticality safety
- Reactor physics
- Radiation shielding
- Advanced/Space reactors
- Thermal hydraulics
- Material and fuel irradiation
- Information/Systems analysis
- Facility safety
- Risk assessment
- Regulatory support
- System instrumentation and controls
- Enrichment technology

FUELS, ISOTOPES, AND NUCLEAR MATERIALS

- Nuclear fuels
- Heavy element production
- Stable/radioactive isotopes
- Medical isotope development
- Separations science and technology
- Nuclear process and equipment design
- Robotics
- Remote handling
- Chemical engineering

Your opportunities at ORNL

- NESLS – Internships in nuclear engineering-related fields
  - Based in Nuclear Science & Technology Division, but not limited too it
  - Highly competitive practicuum
  - www.ornl.gov/sci/nuclear_science_technology/nstip/internship.htm
- SULI – Engineering and Science Internships
  - Less competitive, but only $475/week
  - http://www.scied.science.doe.gov/SciEd/erulf/about.html
- Wigner & Weinberg Fellowships (post-doc)
  - Very prestigious; ~2 per year at ORNL
  - 20% over competitive salary, 2 yrs of research freedom
  - http://jobs.ornl.gov/fellowships/Fellowships.html
- Full-time Staff and Post-Doc Positions
  - http://jobs.ornl.gov/
  - http://www.orau.gov/orise/edu/ornl/postneeds.htm
- The SCALE nuclear analysis code package is inexpensive
  - Source code is free to NE students and faculty
  - A week-long, hands-on training course is only $1800

NESLS	Weekly Stipend
Fourth Year (Senior)	$831
Fifth Year (Graduate)	$968
Masters Completed	$1040

If you only remember one slide…

- **“Because it’s always been done this way,” doesn’t mean it’s right.**
  - **Question everything**

- **Just because it was done before you were born, doesn’t make it wrong.**
  - **Understand WHY it (appears) to work**

- **Be passionate**
  - **Express your passion so that the whole world sees it**

Reactor simulation requires modeling many coupled physics at many scales

Heat Generation

Heat Transport

Thermo-Mechanics

Irradiation Effects

ESBWR

Neutron Transport

Thermal-Hydraulics

Heat Conduction

Isotopic Transmutation

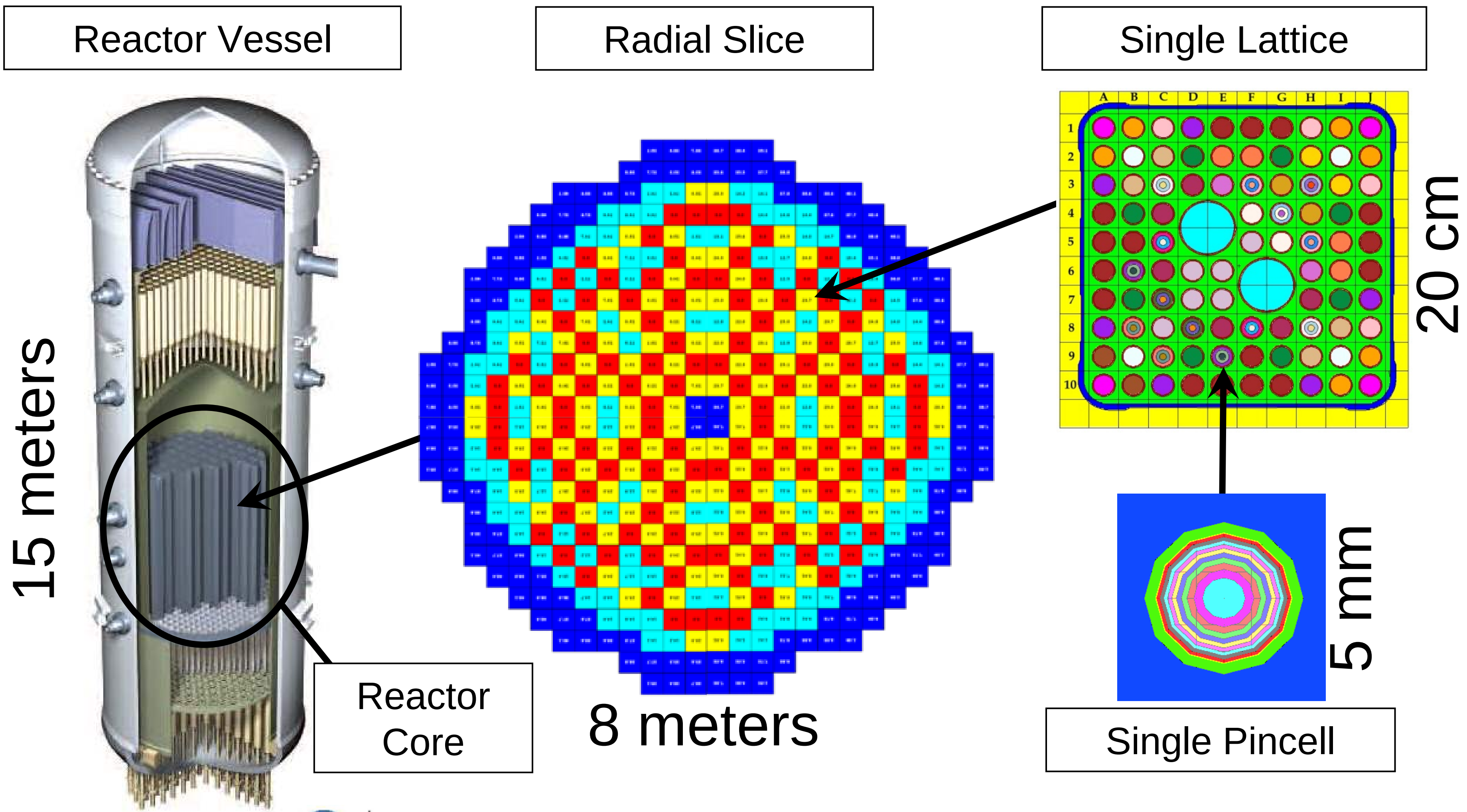
Thermal-Expansion

Irradiation-Induced Swelling

Material Changes

Fuel-, Clad-, Coolant-Chemistry

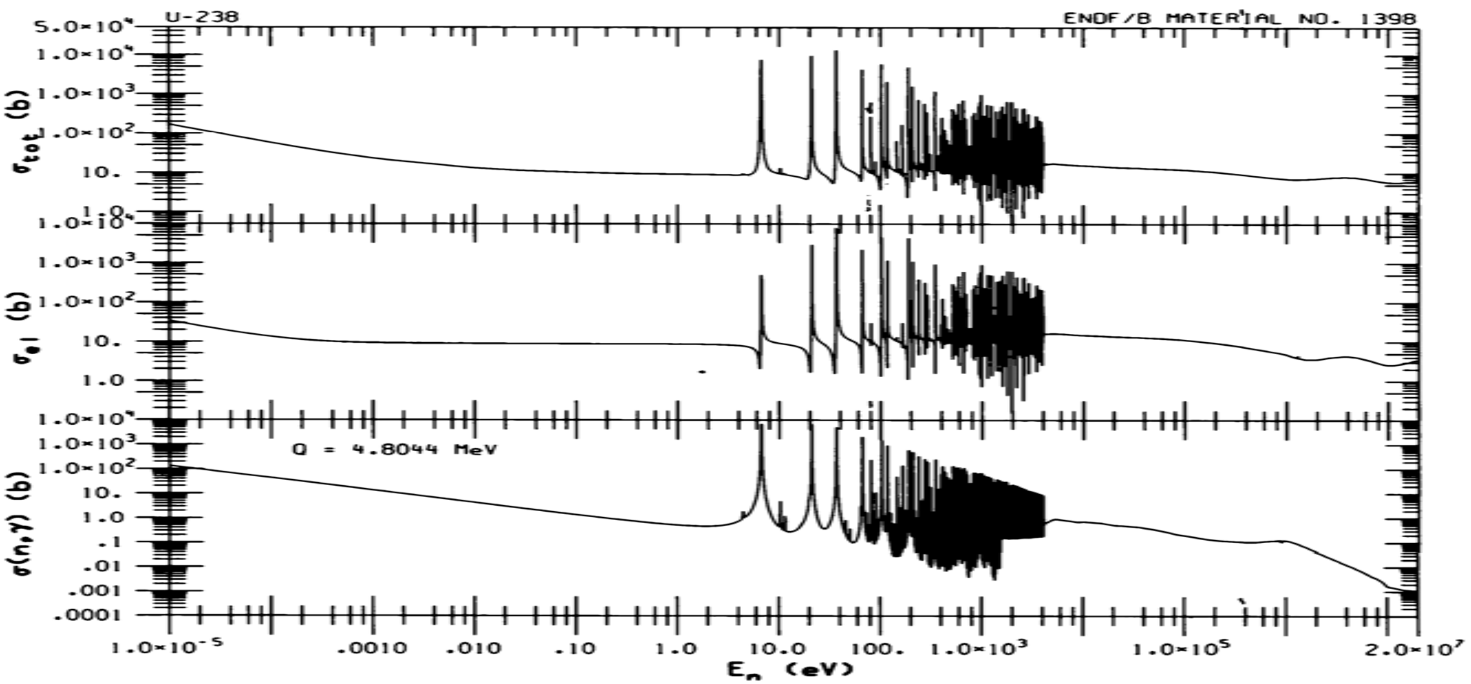
Nuclear reactors are complex systems with a hierarchical structure



ESBWR

Neutron transport: discretizing all space + energy/direction

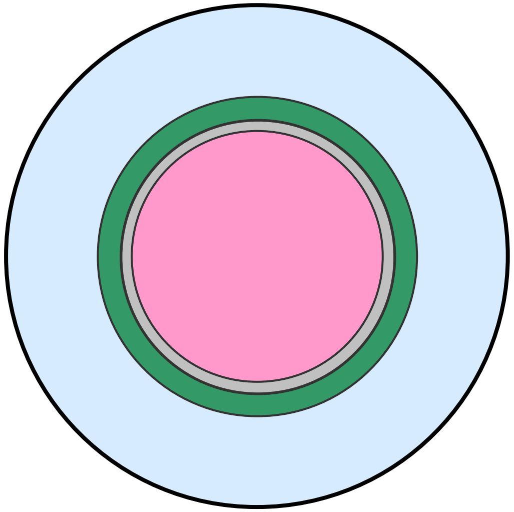
- **Cross section data:**
  - **Defined with 10^6 data-points to describe resonances**
- **We cannot solve a problem with:**
  - **5 orders of magnitude in space**
  - **10^6 degrees of freedom per spatial element**
  - **Plus discretizing the direction of travel**
    - **If you don't know about this, take 602**

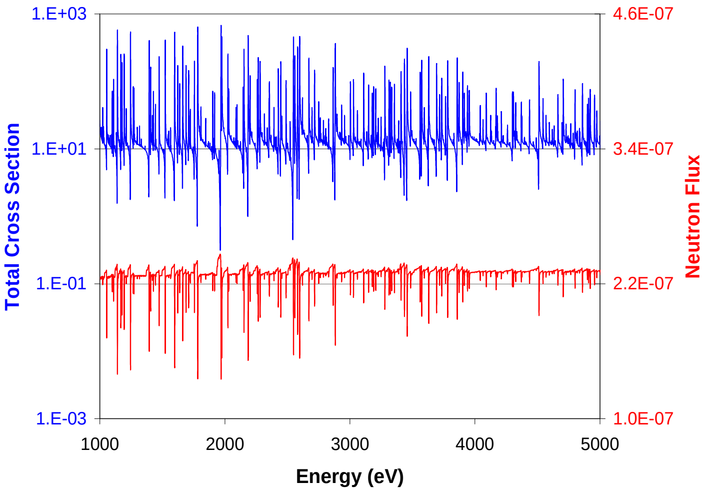


Neutron transport for reactors is modeled with a multi-level approach

- **Level 1: Single Pincell**
  - **High-fidelity 1-D space on a small domain**
  - **High-fidelity in energy**
  - **Approximate BCs and state**

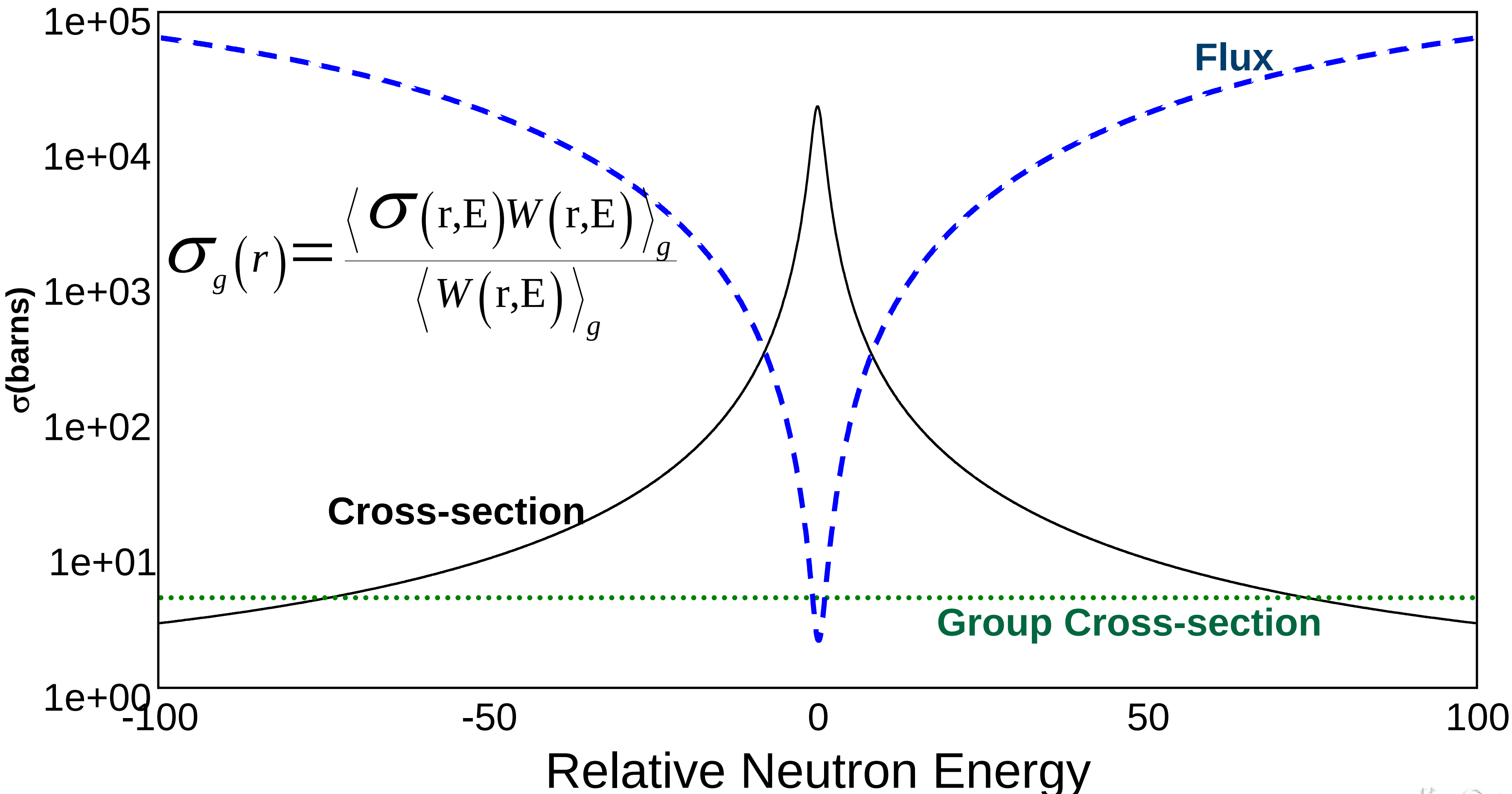
- **Up-scale data to a coarser scale**
  - **Provide “homogenized” or “effective” data**





"Effective" multi-group cross section (σ_g)

- **A weighted average of the continuous cross section (σ)**
- **A weight function (W): usually an approx. to the neutron flux**



$$\sigma_g(r) = \frac{\left\langle \sigma(\mathrm{r,E}) W(\mathrm{r,E}) \right\rangle_g}{\left\langle W(\mathrm{r,E}) \right\rangle_g}$$

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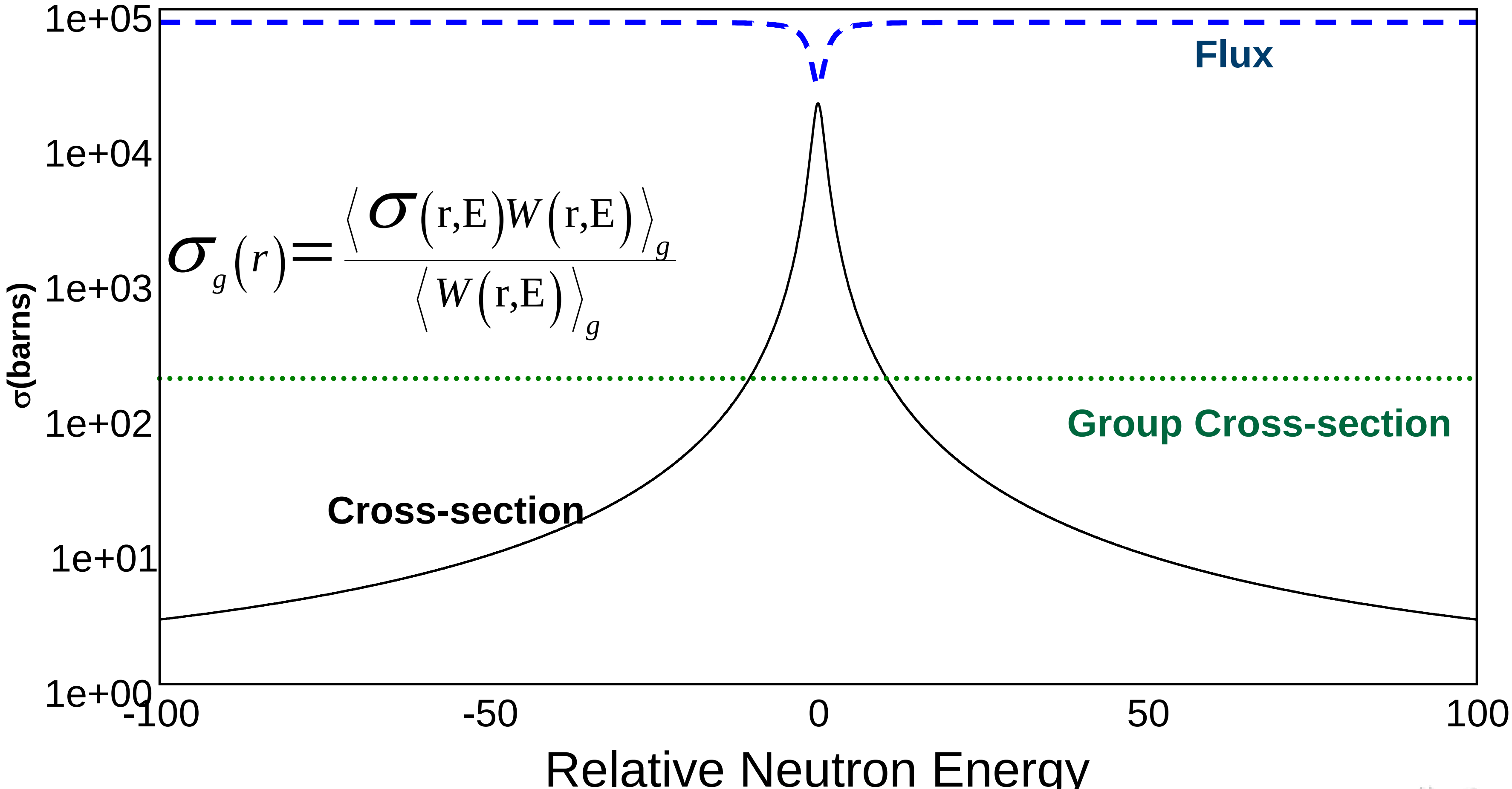

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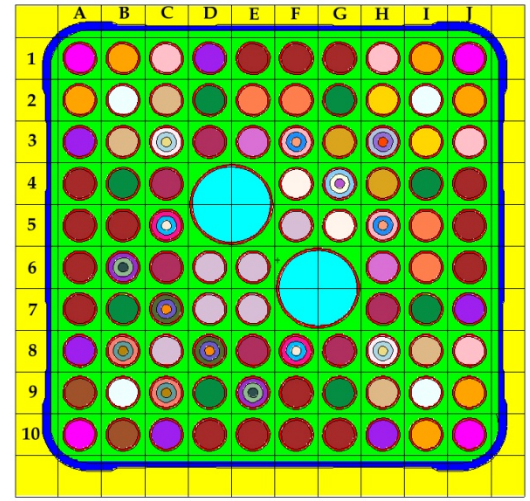
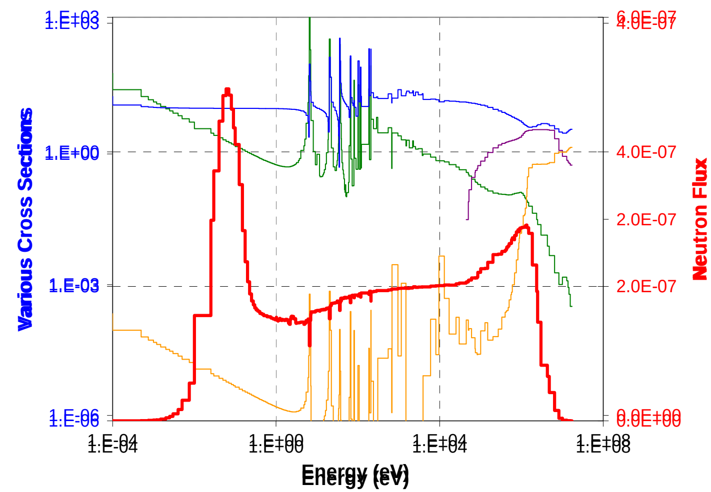
  - **Provide "homogenized" or "effective" data**

- **Level 2: Single Lattice**
  - **Moderate-fidelity 2-D space on a larger domain**
  - **Moderate-fidelity in energy**
  - **Approximate BCs and state**

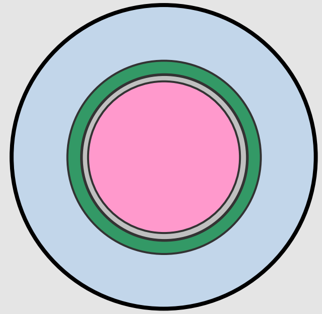
- **Level 3: Full Reactor Core**
  - **Low-fidelity for the full 3-D spatial domain**
  - **Very low-fidelity in energy**
  - **True BCs**
  - **Coupled with other physics for true state**

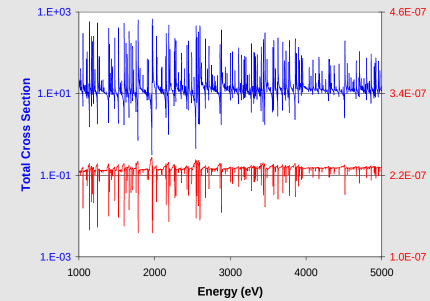


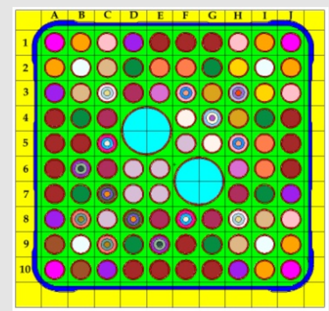


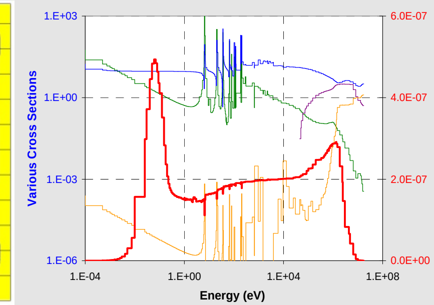
Coupled physics?

- **Level 1 & 2: Lattice Physics**
  - **Pick a geometry**
  - **Pick a thermal-fluid "base state"**
  - **Solve all Level 1's for each Level 2**
  - **Solve Level 2 transport problems**
    - **At a given time (burnup) for the base-state**
  - **Solve depletion equations for a time-step**
    - **Quasi-static time-integration (burnup)**
    - **Upscale data at the base-state for every time-step**
  - **At each time-step, "branch" to a new state**
    - **Upscale data at each branch-point**
    - **Include all branches to cover operational range**

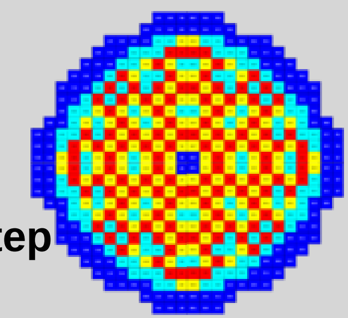


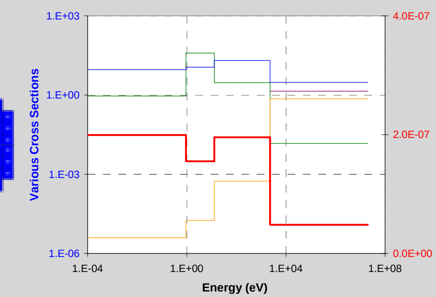






- **Level 3: Core Physics**
  - **Solve coupled T-H/neutronics equations**
    - **T-H is as coarse-grained as neutronics**
    - **Interpolate on "lattice physics" data**
  - **Solve depletion/kinetics equations for a time-step**
    - **Quasi-static time-integration**





Thermal-hydraulics is more empirical (an outsiders view)

- **Level 1: Microscopic level**
  - **Boiling water correlations**
  - **Computational Fluid Dynamics**
- **Level 2: Bundle-level**
  - **Sub-channel simulations (COBRA)**
  - **Non-nuclear experiments**
  - **Power-flow, etc. correlations**
- **Level 3: Full Reactor Core**
  - **"Effective" 1-D T-H with cross-flow simulations**
    - **Embedded with assembly-specific proprietary data**
  - **RELAP, TRAC(E), etc.**

Where are the APPROXIMATIONS?

- **Physics-Based Approximations**
  - **Are we accounting for all of the physics?**
  - **Do we fully account for the fine-to-coarse scale complexity?**
- **Numerical-Based Approximations**
  - **Do the equations model the physics correctly?**
  - **Do we "upscale" from fine-to-coarse consistently?**
  - **Do we couple the physics correctly?**
    - **Even in transients?**
- **Verification-Based Uncertainty**
  - **Are there bugs in the codes? In the input decks?**
  - **Do the codes work together consistently?**
- **Sensitivity/Uncertainty Questions**
  - **Uncertainty in data, numerical convergence**
  - **Is error introduced going between solvers?**
  - **What is the effect on the solution from each error?**
  - **Are the uncertainties coupled?**

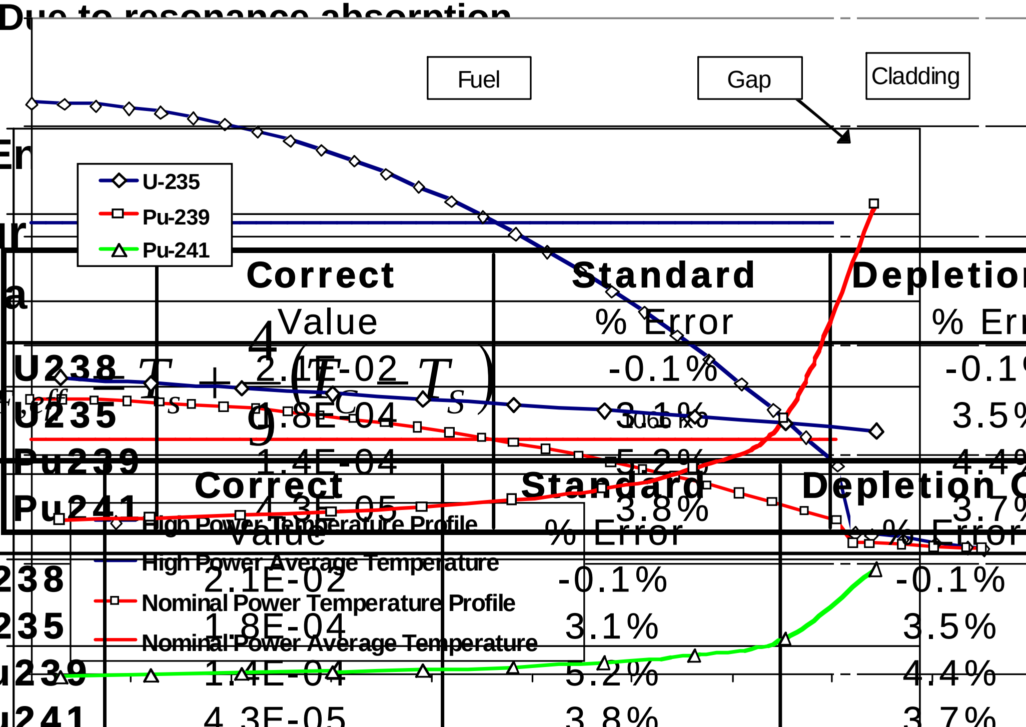
Several quick examples

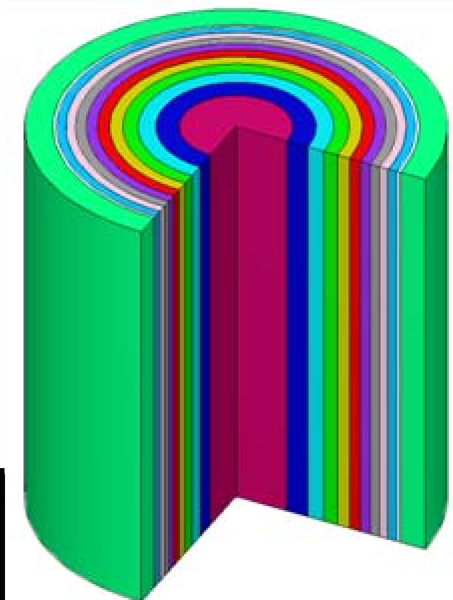
- **Examples:**
  - **Radial depletion and temperature-gradient in fuel**
    - **Do we couple the physics correctly?**
  - **Double-heterogeneity in a burnable absorber**
    - **Are we accounting for the fine-to-coarse complexity?**
  - **Geometric and material changes during burnup**
    - **Are we accounting for all of the physics?**
- **Work in progress:**
  - **Integration of TRITON and NESTLE**
    - **Do we "upscale" from fine-to-coarse consistently**
  - **Sensitivity/uncertainty tools within SCALE**
    - **TSUNAMI and generalized perturbation theory in TRITON**

Radial temperature and depletion profile

- **Approximation:**
  - **"Fuel" is a single composition at a single temperature**
- **Reality:**
  - **Temperature varies radially**
    - **Conductivity in an oxide is small**
  - **Isotopic concentrations varies radially**
    - **Due to resonance absorption**
- **Effect:**
  - **On En**
- **But your**
  - **Use a**

$$T_{Feff} = T_S + \frac{4}{9}(T_C - T_S)$$





	Correct Value	Standard % Error	Depletion Only % Error
U238	2.1E-02	-0.1%	-0.1%
U235	1.8E-04	3.1%	3.5%
Pu239	1.4E-04	5.2%	4.4%
Pu241	4.3E-05	3.8%	3.7%

	Correct Value	Standard % Error	Depletion Only % Error	Effective T % Error
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- **Engineering "fixes" can account for poorly-modeled coupled-physics**

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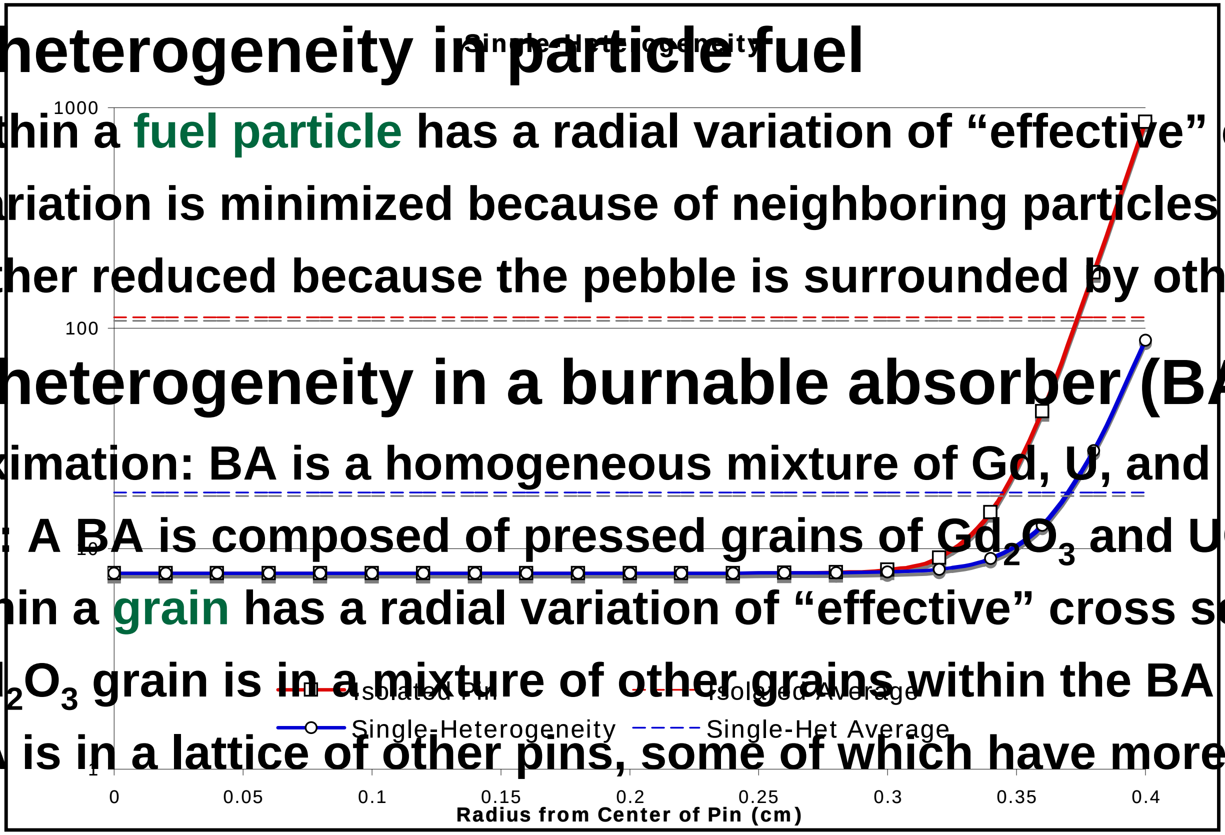
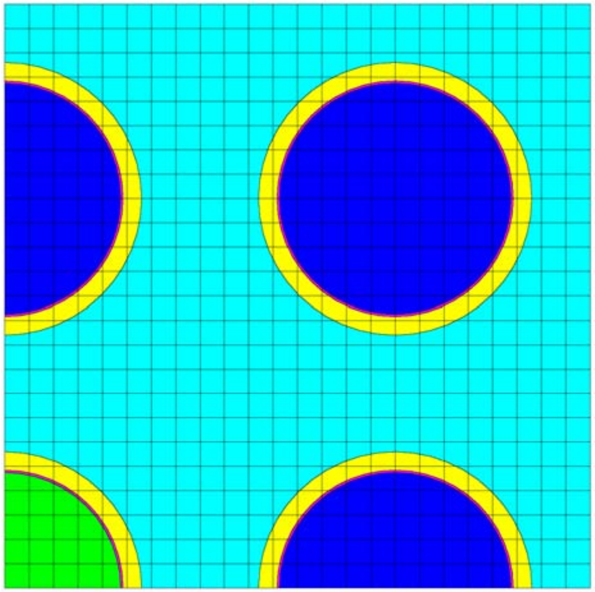
Heterogeneity of a burnable absorber

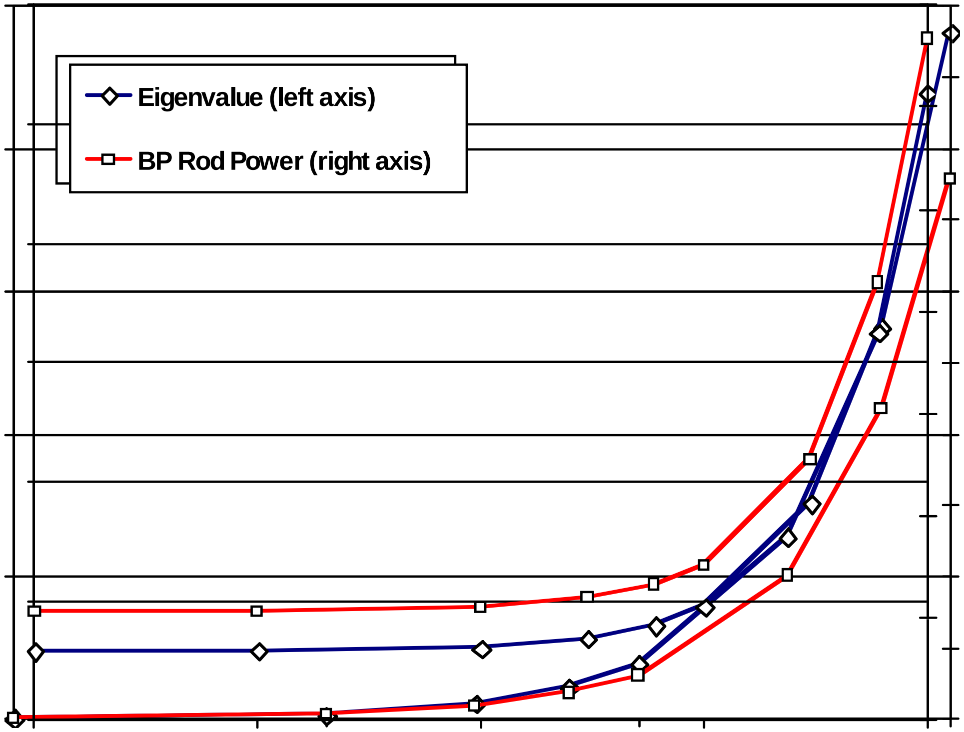
- **Single-heterogeneity**
  - **^{238}U within a pin has a radial variation of the "effective" cross sections**
  - **This variation is minimized because it is in a lattice of other pins with ^{238}U**
  - **CENTRM (1D) calculation accounts for this "single-heterogeneity"**
- **Double-heterogeneity in particle fuel**
  - **^{238}U within a fuel particle has a radial variation of "effective" cross section**
  - **This variation is minimized because of neighboring particles in the pebble**
  - **It's further reduced because the pebble is surrounded by other pebbles**
- **Double-heterogeneity in a burnable absorber (BA)**
  - **Approximation: BA is a homogeneous mixture of Gd, U, and O**
  - **Reality: A BA is composed of pressed grains of Gd_2O_3 and UO_2**
  - **Gd within a grain has a radial variation of "effective" cross section**
  - **The Gd_2O_3 grain is in a mixture of other grains within the BA**
  - **The BA is in a lattice of other pins, some of which have more Gd**



Model: Single BA in a mini-assembly

- **Vary grain-size to determine the double-het effect**
  - **Grain size of 0 is a 'standard' single-het approach**
- **Grains are generally 10-30 microns in diameter**
  - **Microstructure of fuel can effect macro-scale reactor performance, but is small here.**





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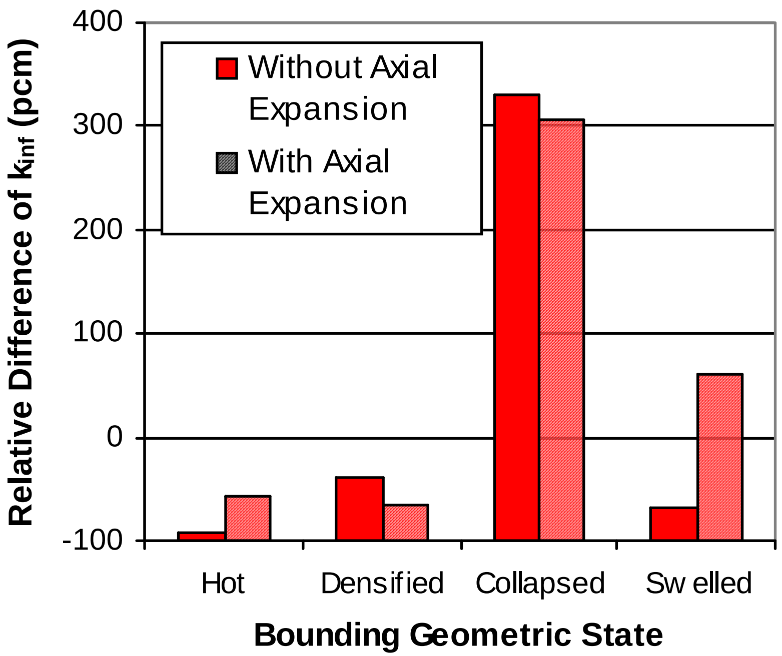
Geometric changes during irradiation

> **Geometric changes in fuel have a measurable, but small, effect on macro-scale reactor performance**

- **Cold:**
  - **As-built geometry of fuel, gap, and cladding**
- **Hot:**
  - **Thermal-expansion (+1%) of clading and fuel (minutes)**
  - **Relative reduction in volume-fraction of moderator**
  - **Axial increase of the active core**
- **Densified:**
  - **Voids in oxide migrate to surface and fuel contracts (-2%) (days to weeks)**
  - **Fuel radius and core height are reduced**
- **Collapsed:**
  - **Pressure from coolant compresses cladding upon fuel (after cycle 1)**
  - **Gap is eliminated, temperature drops**
  - **Relative increase in moderator**
- **Swelled:**
  - **Irradiation-induced swelling leads to fuel expansion (+3.5%) (EOL)**
  - **Relative decrease in moderator**



Fuel and Cladding Chemistry Effects

- **Xenon and krypton:**
  - **Are produced in fuel, migrate to gap and the upper plenum**
  - **Are strong neutron absorbers**
    - **-36 pcm per % of fission gas release (up to 10%)**
  - **Lower the thermal-conductivity of the gap**
    - **Fuel temperature depends on gap-conductance**
- **Corrosion and Crud on outer surface of cladding**
  - **Increases the effective clad diameter, reducing moderator**
  - **Contains absorbing materials**
    - **In BWRs, it has lead to very large axial offsets**
      - **8-12 pcm per micron (up to 100 microns)**
    - **In PWRs, it can contain boron from water**
- **Hydriding in cladding**
  - **Increases moderation due to additional H**
    - **0.4 pcm per ppm of H (up to 1000 ppm)**
- **These are mostly localized errors that are small in a global sense**

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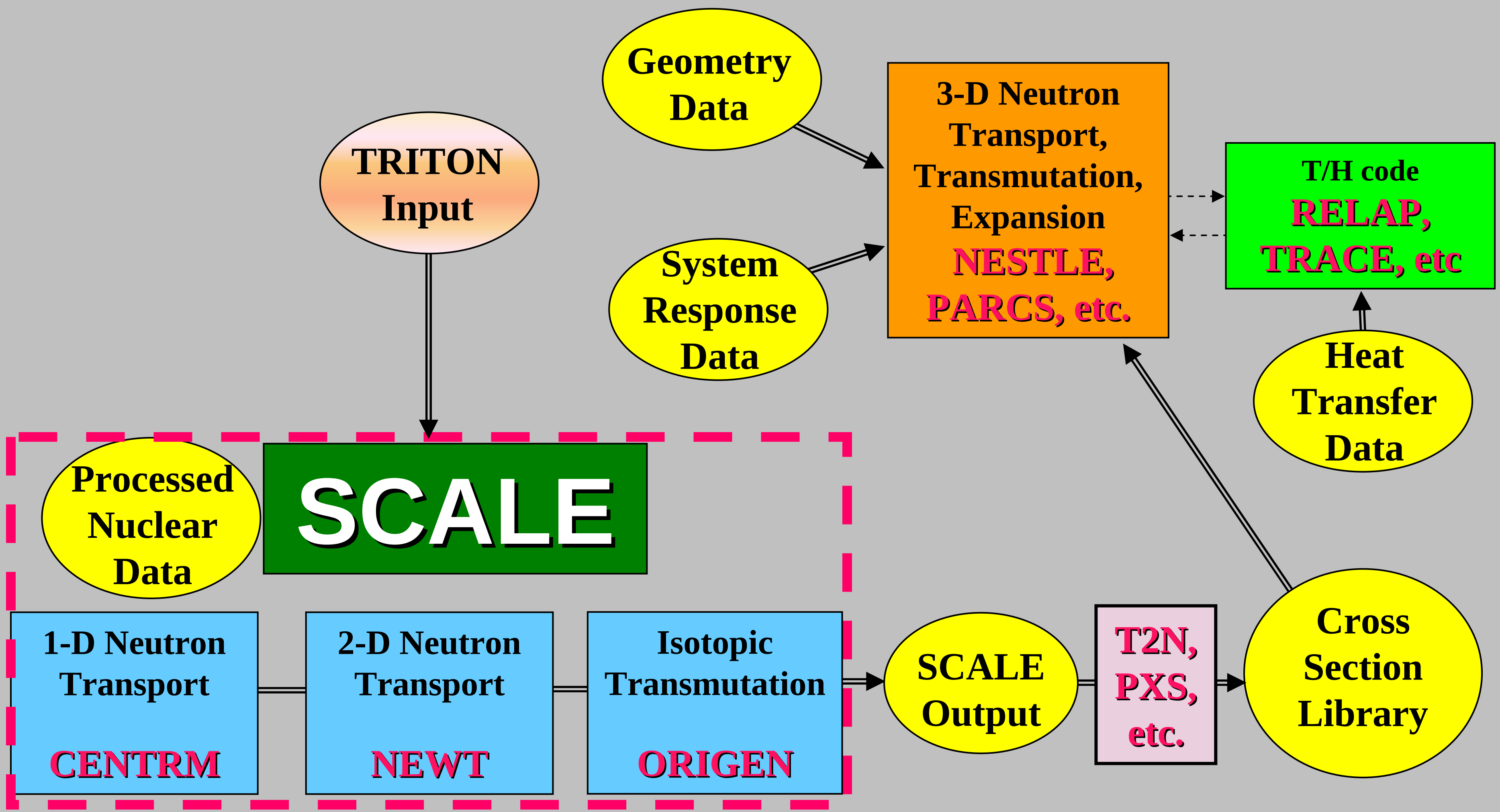
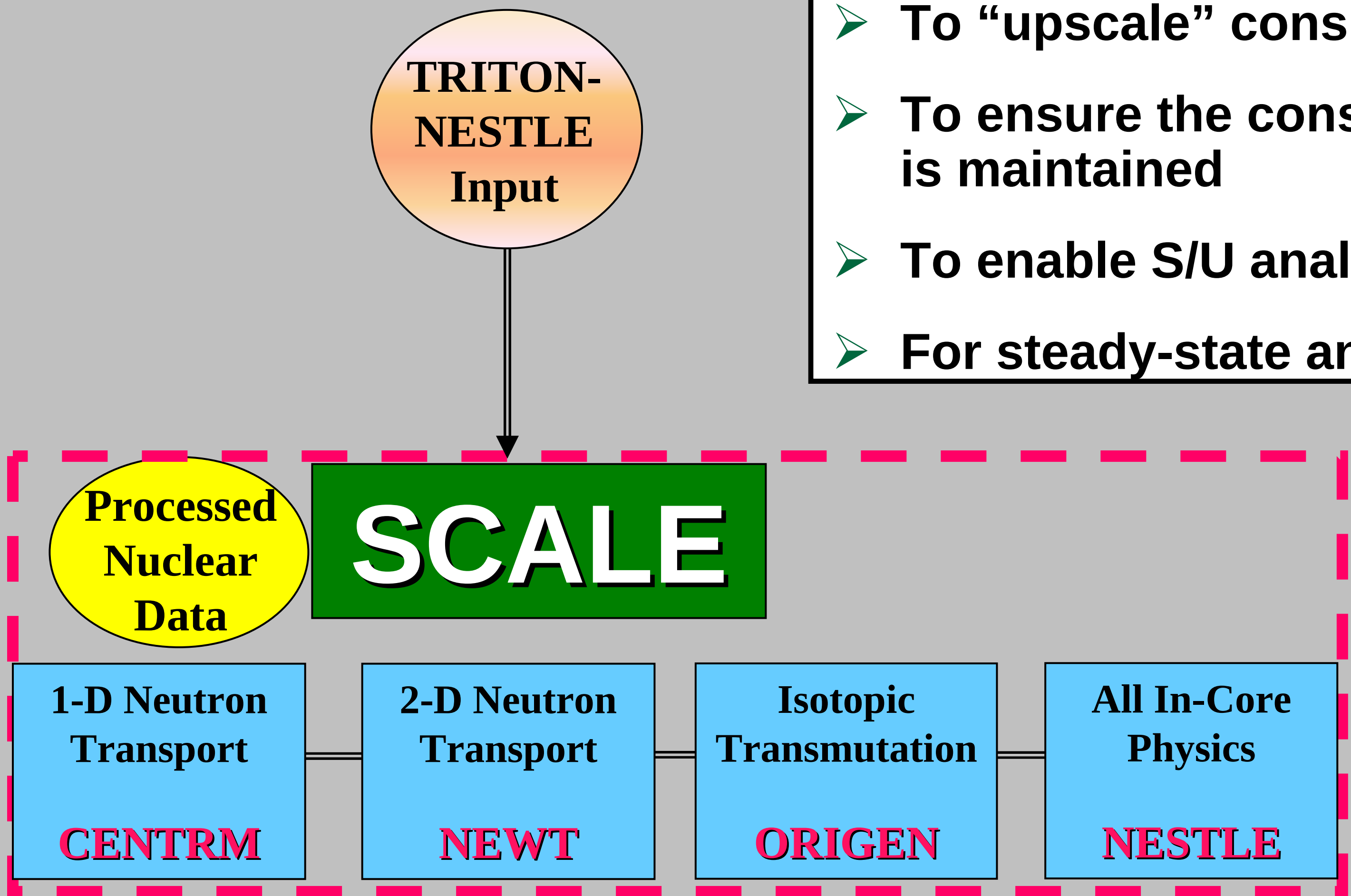
End-to-End reactor analysis with open-source codes is difficult

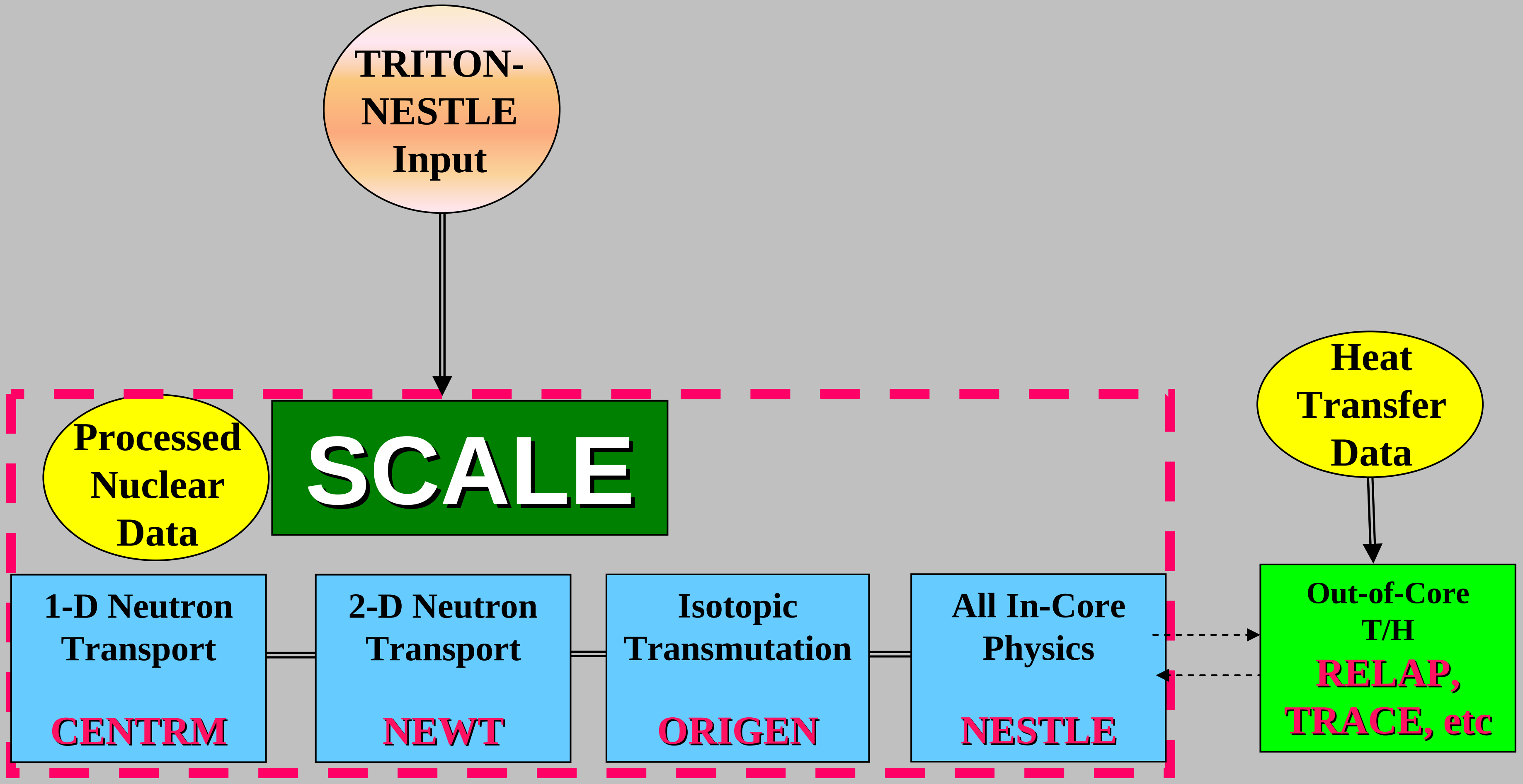


NESTLE is being integrated with SCALE to make the whole process easier

- To "upscale" consistently
- To ensure the consistency is maintained
- To enable S/U analysis
- For steady-state analyses



Perhaps in the future it could be extended to transients?



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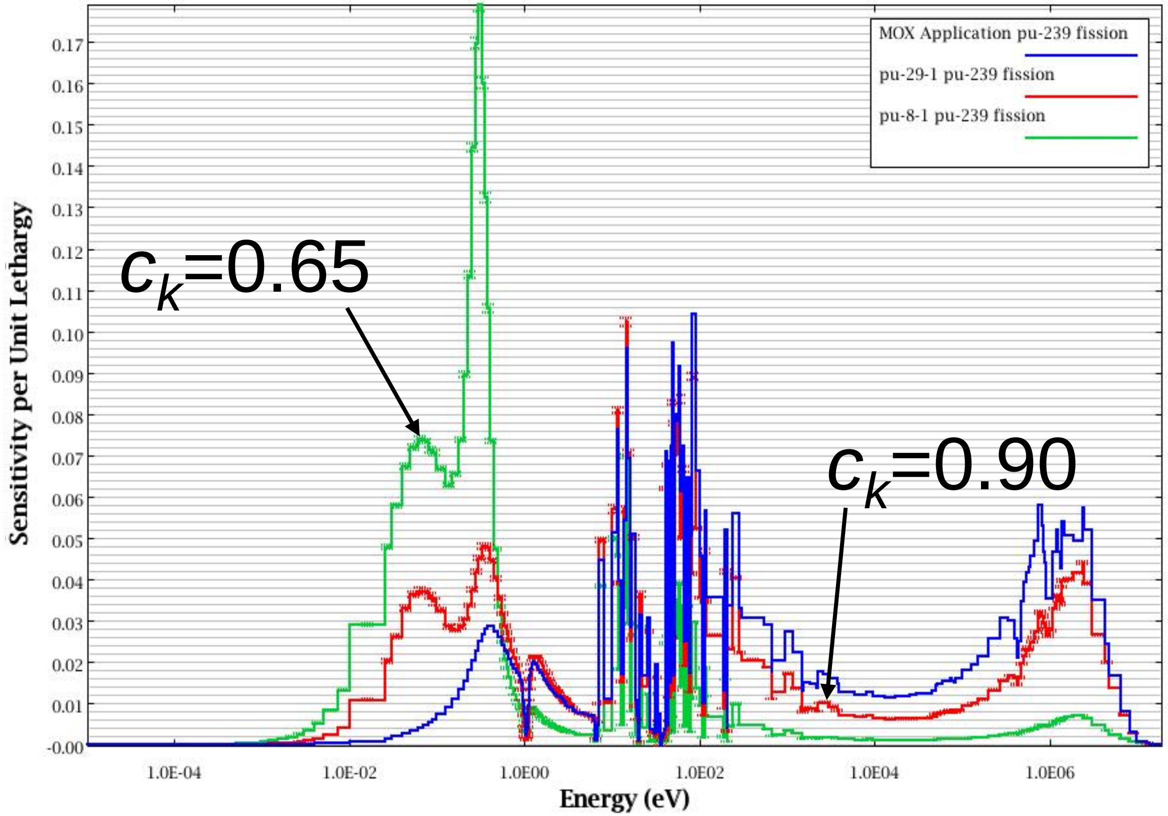
TSUNAMI: Tool for S/U Analysis with XSDRN (1-D) and KENO-VI (3-D)

- **Determination of critical experiment benchmark applicability to nuclear criticality safety analyses**

- **The design of critical general physics experiments (GPE)**

- **The estimation of computational biases and uncertainties for the determination of safety subcritical margins**

^{239}Pu Fission Sensitivity Profiles: Sensitivity of k_{eff} to cross-section



Conclusions

- **"Because it's always been done this way," doesn't mean it's right.**
  - **Do we couple the physics correctly?**
  - **Are we accounting for the fine-to-coarse complexity?**
  - **Are we accounting for all of the physics?**
  - **Do we "upscale" from fine-to-coarse consistently?**
- **Just because it was done before you were born," doesn't make it wrong.**
  - **Engineering "fixes" can account for poorly coupled physics**
  - **Effects of fuel microstructure and geometric/material changes are small**
    - **Disclaimer: For existing LWRs with less than 5% enriched UO_2 fuel, etc…**
    - **These ASSUMPTIONS should not extend beyond this limited knowledge basis**
- **Be passionate about whatever you do**
  - **Nuclear energy should be the primary solution for US energy needs**
  - **But we are restrained by a limited knowledge basis**
  - **There is much to be learned and new resources available**

What resources?

- **Interdisciplinary Research**
  - **We need to move away from "transport people" and "T-H experts" to work and learn together**
    - **Our physics aren't separable, and we shouldn't be either**
- **Mathematicians**
  - **Great progress has been made with Krylov solvers, finite-element methods, wavelet-basis functions, multi-grid acceleration, etc.**
    - **Transfer the technology they developed to nuclear engineering**
- **Open-source Software and Tools**
  - **Use them:**
    - **LAPACK, VisIt, MPI, HDF5, OpenMP, DOXYGEN, ZOLTAN, CUBIT, Metis, PETSc, Python, or their equivalent**
  - **If you're writing code and don't know what these are, find out**
- **Big Computers**
  - **The age of faster processors is gone - accept it - 3 GHz is it.**
    - **Learn how to write code for parallel chips and clusters**