Modern, High Performance Transport and Thermal-Hydraulics Codes at LLNL

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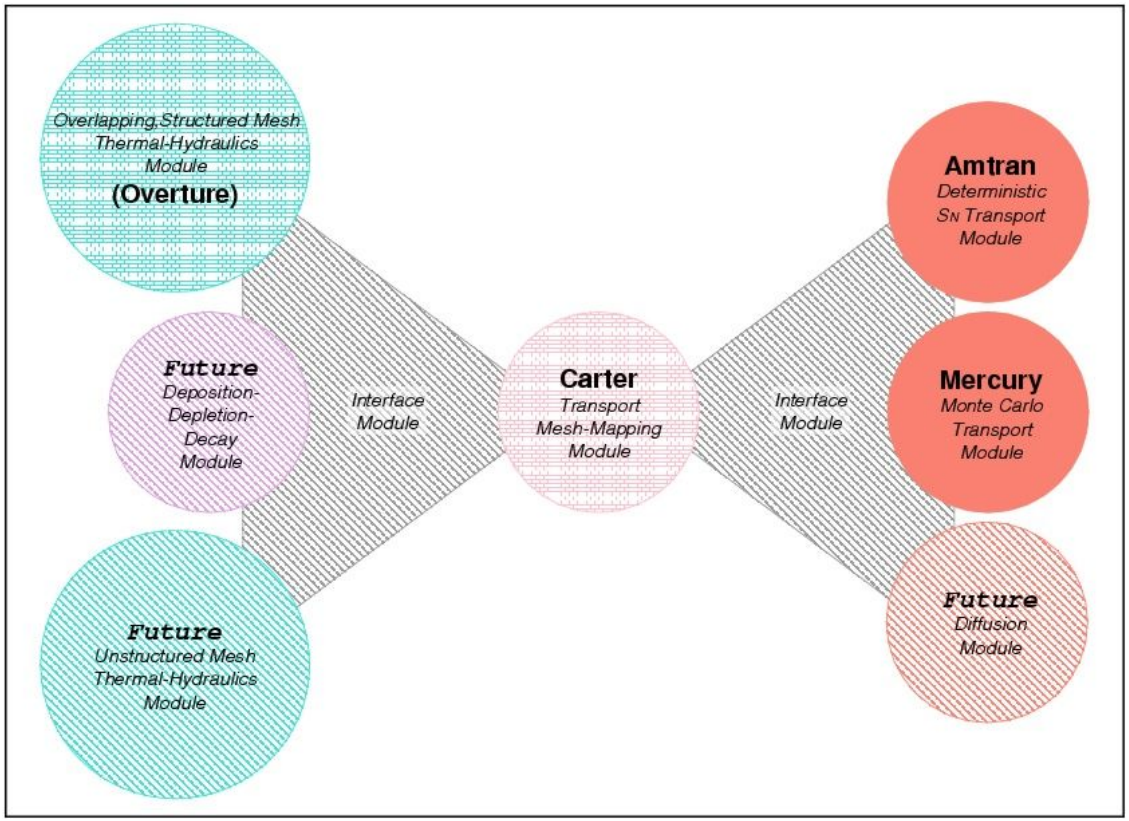
A New Beginning for Reactor Analysis Codes at LLNL

- Development of a high-performance, coupled, multi-physics reactor analysis code is getting underway at LLNL with LDRD funding.
- This effort leverages mature code development activities which have been underway for more than a decade.

Schematic Layout of the LLNL Coupled, Multi-Physics Reactor Analysis Code



Modern Particle Transport Codes at LLNL

- Modern particle transport codes have been developed at LLNL over the past decade as part of the Advanced Simulation and Computing (ASC) program:
  - ***Amtran***: A discrete ordinates S_N (deterministic) particle transport code
    (Project Leader: *Chris Clouse* – clouse1@llnl.gov)
  - ***Mercury***: A Monte Carlo (stochastic) particle transport code
    (Project Leader: *Rich Procassini* – spike@llnl.gov)
  - ***Carter:*** A mesh-mapping code for transport mesh flexibility
    (Project Leader: *Jeffrey Grandy* – grandy1@llnl.gov)
- These codes were designed and developed for high-performance computing applications which require:
  - Very-large problem domains in space, energy, angle and time $\phi(\vec{r}, E, \hat{\Omega}, t)$
  - Solution on a wide variety of parallel computing platforms, using both message-passing and shared-memory data communication methods:
    - ➔ PCs → SMP nodes → Clusters → MPPs (such as Purple and BlueGene/L)

The *Amtran* S_N Transport Code

- `Status` → **Amtran** is a *production ready* code which:
  - Has undergone ~30 person-years of development
  - Has been V&V for a wide variety of applications
  - Runs efficiently on a *very* diverse set of serial and parallel computing platforms
  - Is an 'export controlled' code (true for *all modern* neutron transport codes)
  - Reference: Clouse, C. J., *Parallel Deterministic Neutron Transport with AMR*, in Computational Methods in Transport, edited by Graziani, F.R., Springer-Verlag, Pages 499 - 512 (2006).
- `Capabilities` → The features of the **Amtran** S_N code include:
  - Time dependent or static transport of neutrons (n) and gammas (γ)
  - Finite element treatment of angular fluxes
  - Support for 1-D spherical (radial), 2-D *r-z* cylindrical and 3-D Cartesian meshes
  - Variable spatial resolution via the Adaptive Mesh Refinement (AMR) method
  - Variable angular resolution via the Adaptive Directional Refinement (ADR) method

The *Amtran* S_N Transport Code *(continued)*

- `Capabilities` *(continued)* →
  - Static k_{eff} and α eigenvalue criticality calculations for neutrons
  - Multi-group treatment of cross sections
  - Thermal up- or down-scattering model
  - Thermally-broadened cross sections with *no* temperature-bin interpolation
  - Delayed neutron emission
  - Criticality probability method for estimating the probability of a chain reaction
  - Complete parallelization of phase space is supported:
    - Message-passing (MPI) decomposition over both spatial domains and energy groups $(\vec{r}, E)$
    - Shared-memory threading (Open-MP) over discrete ordinates (rays / angles) $(\hat{\Omega})$
    - Spatial load balancing via (static) domain overloading

The *Mercury* Monte Carlo Transport Code

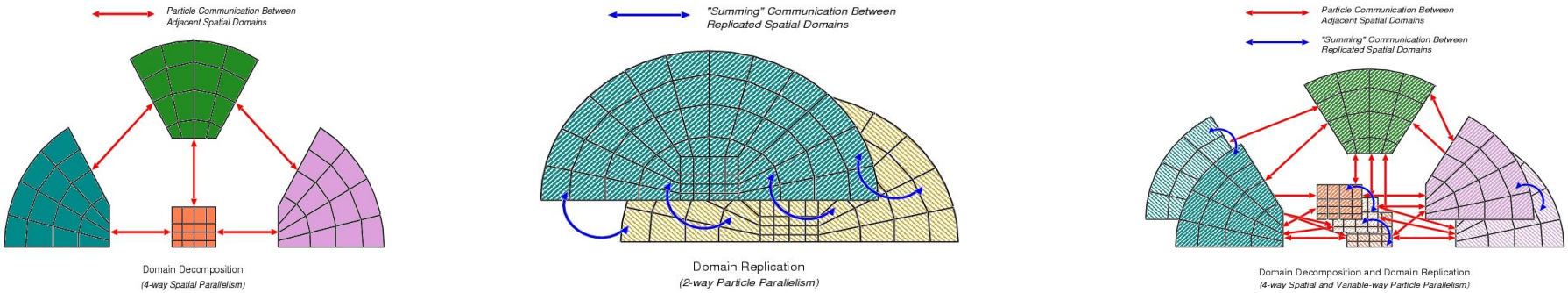
- `Status` → **Mercury** is a *production ready* code which:
  - Has undergone ~30 person-years of development
  - Has been V&V for a wide variety of applications
  - Runs efficiently on a *very* diverse set of serial and parallel computing platforms
  - Is an 'export controlled' code (true for *all modern* neutron transport codes)
  - References: See the **Mercury** web site → http://nuclear.llnl.gov/mercury
- `Capabilities` → The features of the **Mercury** Monte Carlo code include:
  - Time dependent or static transport of neutrons (n), gammas (γ) and light charged ions $({}^{1}H, {}^{2}H, {}^{3}H, {}^{3}He, {}^{4}He)$
  - Particle tracking through a wide variety of problem geometries:
    - *Mesh:* 1-D spherical (radial), 2-D *r-z* structured and quadrilateral unstructured, 3-D Cartesian structured and tetrahedral unstructured
    - *Non-Mesh:* 3-D combinatorial geometry

The *Mercury* Monte Carlo Transport Code *(continued)*

- `Capabilities` *(continued)* →
  - Static k_{eff} and α eigenvalue criticality calculations for neutrons
  - Dynamic α calculations for all types of particles
  - Multi-group and continuous energy treatment of cross sections
  - Thermal up- or down-scattering model
  - Thermally-broadened cross sections with *linear* temperature-bin interpolation
  - Deposition of energy, plus isotope depletion / production via nuclear reactions
  - Criticality probability method for estimating the probability of a chain reaction
  - Support for general sources and tallies

The *Mercury* Monte Carlo Transport Code *(continued)*

- `Capabilities` *(continued)* →
  - A flexible, hybrid approach to parallelism is supported:
    - ➔ *Domain Decomposition:* Spatial parallelism via message passing (MPI)
    - ➔ *Domain Replication:* Particle parallelism via message passing (MPI)



    - ➔ *Task Decomposition:* Particle parallelism via shared-memory threads (Open-MP)
  - These methods may be used individually or in combination
  - Two forms of dynamic load balancing are supported. Each responds to particle workload in an effort to achieve efficient parallel calculations:
    - ➔ *Dynamic Replication:* Dynamic, variable assignment of processors to domains
    - ➔ *Dynamic Decomposition:* Dynamically sized spatial domains

The *Carter* Mesh Mapping Code

- `Status` → **Carter** is a *production ready* code which:
  - Has undergone ~5 person-years of development
  - Runs efficiently on a *very* diverse set of serial and parallel computing platforms
- `Capabilities` → The features of the **Carter** mesh mapping code include:
  - Second-order accurate mapping of mesh-based fields between a *general donor* (thermal-hydraulics) mesh to a *structured target* (transport) mesh
  - Permits efficient, coupled, multi-physics calculations via different / optimal meshes for the thermal-hydraulic and transport modules:
    - Disparate donor / target mesh types (connectivities)
    - Disparate donor / target mesh resolutions
  - Parallel computations are supported via:
    - Spatial domain decomposition
    - Static load balancing

Modern Thermal-Hydraulics Codes at LLNL

- A modern thermal-hydraulics codes is being developed at LLNL within the **Overture** framework, which has been developed with support from the DOE Office of Science.
  (Project Leader: *William Henshaw* – henshaw@llnl.gov)
- `Status` → **Overture** is a *near-production quality* code framework which:
  - Has undergone >10 person-years of development
  - Has been used to model diverse physics: flow, heat transfer, electromagnetics, etc.
  - Reference: See the **Overture** web site → http://www.llnl.gov/CASC/Overture
- `Capabilities` → The features of the **Overture** code framework include:
  - Solving coupled sets of PDEs on overlapping, structured (overset) meshes.
  - Incompressible flow and thermal transfer modules are being integrated to produce a thermal-hydraulics (T-H) module.
  - High accuracy, parallel multi-grid PDE solvers are under development for use by the T-H module.
  - Flexible restart capabilities are currently limited and need to be extended.

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