CESAR: Overview of Deep Dive

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CESAR Challenge: Predict Pellet-by-Pellet Power Densities and Nuclide Inventories for the Full Life of Reactor Fuel (~5 years)

CESAR physics

- Computational Fluid Dynamics (Conjugate Heat Transfer)
- Neutron Transport
- Fully Coupled CFD/Transport

- CESAR focuses on nuclear reactor flows and physics (neutron transport) calculations
  - Accurate simulations have always been an integral part of design, licensing, and optimization of nuclear reactors
  - Innovative reactor designs require far more physics fidelity than current methods provide
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  - Accurate simulations have always been an integral part of design, licensing, and optimization of nuclear reactors
  - Innovative reactor designs require far more physics fidelity than current methods provide
- However, many of the co-design issues are of more general relevance to
  - **Incompressible CFD**
  - **Neutral particle transport**

**Three codes are focus of CESAR research**

- **Computational Fluid Dynamics**
- **Neutron Transport** (approach 1)
- **Neutron Transport** (approach 2)

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- **Incompressible Navier-Stokes**
- **Boltzmann**
- **Stochastic (Monte Carlo)**

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- **Spectral Elements**
- **Method of Characteristics**
- **Data and Domain Decomposition**
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- Computational Fluid Dynamics
  - Incompressible Navier-Stokes
  - Spectral Elements
  - Nek
- Neutron Transport (approach 1)
  - Boltzmann
  - Method of Characteristics
  - UNIC
- Neutron Transport (approach 2)
  - Stochastic (Monte Carlo)
  - Data and Domain Decomposition
  - OpenMC
  - Proxy Apps
    - High FLOP/load ratios
    - Nearest neighbor
    - Bulk synchronous
    - Low memory per node required for scalability
    - Global AllReduce latency key
    - Load dominated
    - Branch heavy
    - Highly parallelizable in particle space
    - Poor locality in x-section and tally space
    - Low FLOP/s rate
    - Performance hot spot

Categories of Proxy-apps

- **Kernels**
  - A standalone faithful representation of a performance critical component whose behavior does not qualitatively change when interoperating with other components

- **Micro-apps**
  - Components that cannot have a meaningful standalone representation in a minimal combination with other components

- **Mini-apps**
  - Reduced instantiation of application configurations that exercise the interoperability

Organization of Proxy Apps

- Each class of proxy-apps has its own webpage
  - Download
  - Quick start guides (README files)
    - Instructions to build and run
    - Parameters that affect the run
    - Verification data
    - Example configuration
  - Links for
    - Publications related to the whole application
    - Technical reports of findings and acquired wisdom
    - Discussion forum

http://cesar.mcs.anl.gov/content/software

Possible Limitations

- **Proxy-apps** inherently have the implementation bias built into them
  - Data structures
  - Control flow
  - Communication pattern

- Some way to represent the basic computation without the bias would provide more insight

- Ample verification studies needed

- Provision for embedding algorithmic innovations for exascale in the proxy-apps
Four CESAR deep dive talks

- Monte Carlo neutronics (Siegel)
- Incompressible CFD (Elia Merzari)
- Deterministic Transport (Micheal Smith)
- Neutronics/CFD coupling (Tim Tautges)