Applied mathematics in nuclear science and engineering

S. V. G. Menon

Theoretical Physics Division

Bhabha Atomic Research Centre

17/08/2007 10:00 PM

Theoretical and computational modeling

- Research in Nuclear Science- main mandate of BARC
  - Basic science
  - Design of new reactors and systems
  - Applications of nuclear energy in other fields

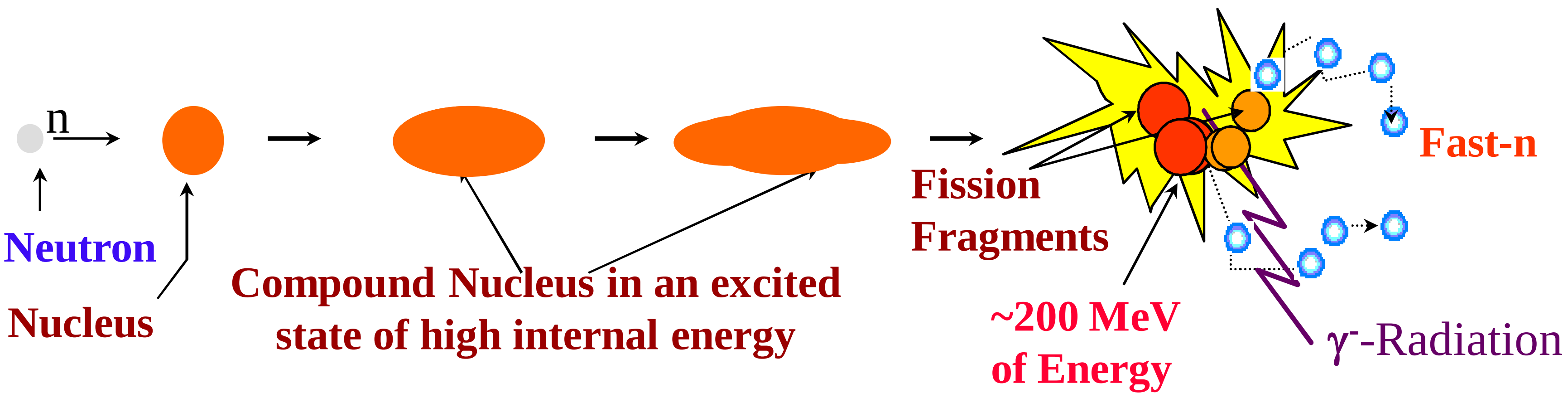
- Tasks of theoretical physicists
  - Theoretical research in the physical processes
  - Develop mathematical models and computing methods
  - Implement & apply to design, analysis and operation

- Research in new methods for simulations
  - Simulations of more details of systems
  - Simulations involving multi-physics models
  - Develop new methods for parallel computing systems

Topics for today

- Modeling neutron distributions in fission reactors
- Radiation–hydrodynamics of high-temperature plasmas
- Two-fluid description of plasmas in fusion reactors

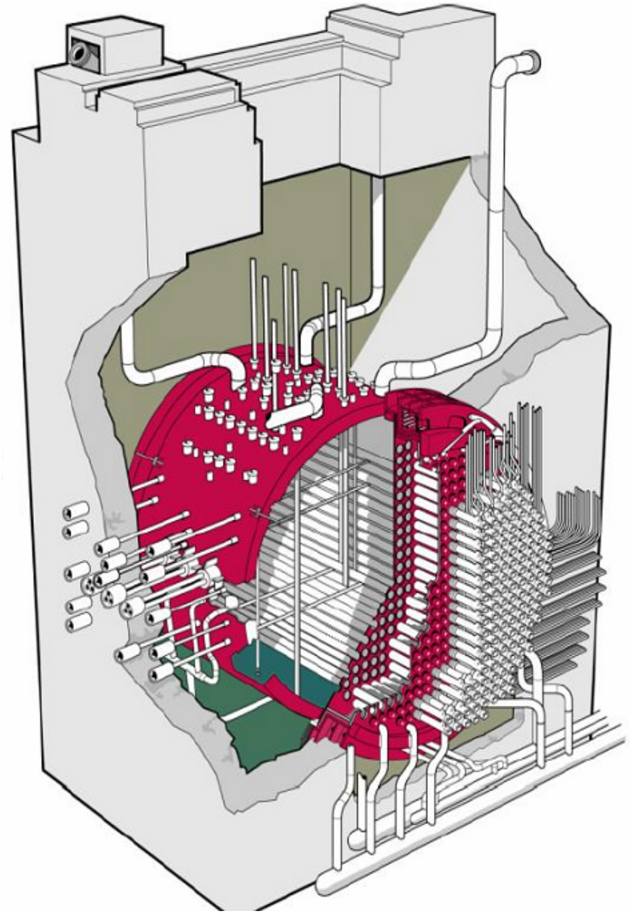
Nuclear fission



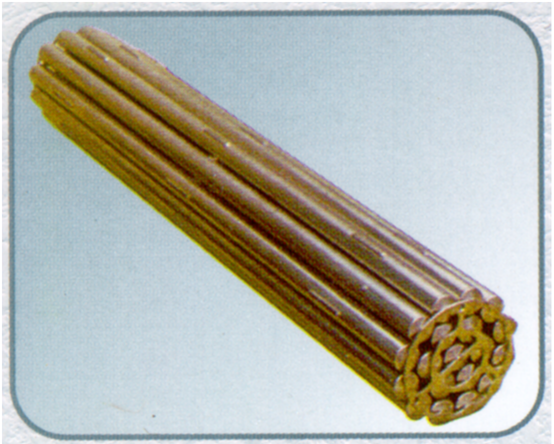
$$_{92}U^{235} + {}_{0}n^{1} \longrightarrow {}_{36}Kr^{92} + {}_{56}Ba^{141} + 3({}_{0}n^{1}) + \text{Energy (200 MeV)}$$

$$_{92}U^{235} + {}_{0}n^{1} \longrightarrow {}_{42}Mo^{95} + {}_{57}La^{139} + 2({}_{0}n^{1}) + \text{Energy (200 MeV)}$$

Pressurized heavy water reactor core



- Pressurized heavy water reactor core
- Total of 306 fuel channels, which contain 12 fuel assemblies per channel, each with 19 fuel pins
- Coolant flows between the elements and removes energy



19 element PHWR fuel assembly

Neutron distribution in reactors

- Neutrons and the nuclei form a binary mixture.
  - Density of nuclei ~ 10^{22} / C.C.
  - Density of neutrons ~ 10^{9} / C.C.
  - Neutron-neutron collisions are negligible

- Boltzmann transport equation for neutron flux:

$$\frac{1}{v}\frac{\partial}{\partial t}\psi + \vec{\Omega}\cdot\nabla\,\psi(\vec{r},\vec{\Omega},E,t) + N(\vec{r},t)\,\sigma(\vec{r},E)\,\psi(\vec{r},\vec{\Omega},E,t) =$$
$$\int\int N(\vec{r},t)\,\sigma(\vec{r},E'\to E,\vec{\Omega}\cdot\vec{\Omega}')\,\psi(\vec{r},\vec{\Omega}',E',t)\,dE'\,d\vec{\Omega}' + S(\vec{r},\vec{\Omega},E,t)$$

  - Equation in seven variables

- All nuclear cross-sections are either measured or computed from nuclear models

Discrete ordinates method

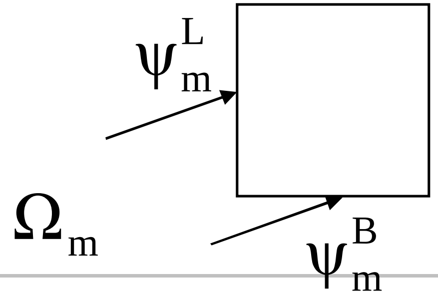
- The time derivative is approximated using the Euler backward scheme, to ensure stability
- Energy variable ($0 \leq E \leq 20$ MeV) is divided into a large number (~ few hundred) of groups:
- The continuous variable Ω is replaced by a discrete set:

$$\int \psi(\Omega)\, d\Omega = \sum_m \omega_m \, \psi_m$$

- These approximations converts the transport equation into a PDE:

$$\Omega_m \bullet \nabla \psi_m + \sigma\, \psi = \sum_m \omega_m \, \psi_m + S_m$$

- The standard approach is then to solve this equation in a cell or mesh using a FD or FEM approximation



The diffusion approximation

- Transport equation is reduced to the diffusion equation, when the angular distribution is nearly isotropic:

$$\varphi(\vec{r},E,t) = \int \psi(\vec{r},\Omega,E,t)\,d\Omega$$

- To use the diffusion equation, it is necessary to smear out the heterogeneities – a sort of coarse graining

$$\frac{1}{v}\frac{\partial}{\partial t}\phi + \nabla \cdot D(\vec{r},E,t)\,\nabla\,\phi(\vec{r},E,t) + N(\vec{r},t)\,\sigma(\vec{r},E)\,\phi(\vec{r},E,t) =$$

$$\int N(\vec{r},t)\,\sigma(\vec{r},E' \to E)\,\phi(\vec{r},E',t)\,dE' + S(\vec{r},E,t)$$

- Numerical schemes for diffusion equation are used in simulations (FDM, FEM, Nodal methods, etc)

Nature of problems

- Uncontrollable errors introduced in coarse graining
- Solution needed in multi-dimensional geometries

- Stability of numerical schemes
  - Time differencing
  - Stiff equations

- Generalized eigenvalue problems – steady state

$$A\,\vec{\phi}_n = \frac{1}{\lambda_n} F\,\vec{\phi}_n$$

  - A $\rightarrow$ Diffusion matrix
  - F $\rightarrow$ Fission matrix
  - $\lambda_n \rightarrow$ Eigenvalues
  - λ_1 = Multiplication factor

Sparse Matrix Methods

Simulation problems

- Time dependent problems
  - Need to control errors and stability
  - Incorporating feedback - temperature effects, fuel depletion, etc
- Steady state solutions
  - Large sparse systems
  - Iterative solution methods
    - Acceleration of convergence
- Coupling of neutron diffusion to thermal hydraulics
  - Heat transfer
  - Postulated accidental scenarios

An inverse problem

- Xe^{135} and Sm^{149} induced power oscillations occur in large pressurized heavy water reactors

- Using measured neutron flux at several locations, the reactor power has to be kept steady.

- This leads to an inverse problem –
  - The spatial distribution of neutron absorbers is determined from measured flux
  - This has to be done on-line for uninterrupted reactor operation

More recent algorithms

- Conjugate gradient and related Krylov-space methods

$$\{\vec{r}_0, A\vec{r}_0, A^2\vec{r}_0, A^3\vec{r}_0, \ldots\ldots A^{i-1}\vec{r}_0\}, \vec{r}_0 = b - A\vec{x}_0$$

  - Use of pre-conditioners
  - Needs only vector-matrix products
  - Efficient parallel algorithms

Conjugate gradient

Bi-conjugate gradient

Generalized minimum residual

- Jacobian-free Newton-Krylov methods

$$F(u) = 0$$

$$J_k\ \delta u_k = -F(u_{k-1}),\ u_k = u_{k-1} + \delta u_k$$

$$J_k\ v \approx \frac{1}{\varepsilon}[F(u_{k-1} + \varepsilon\ v) - F(u\ \ )]$$

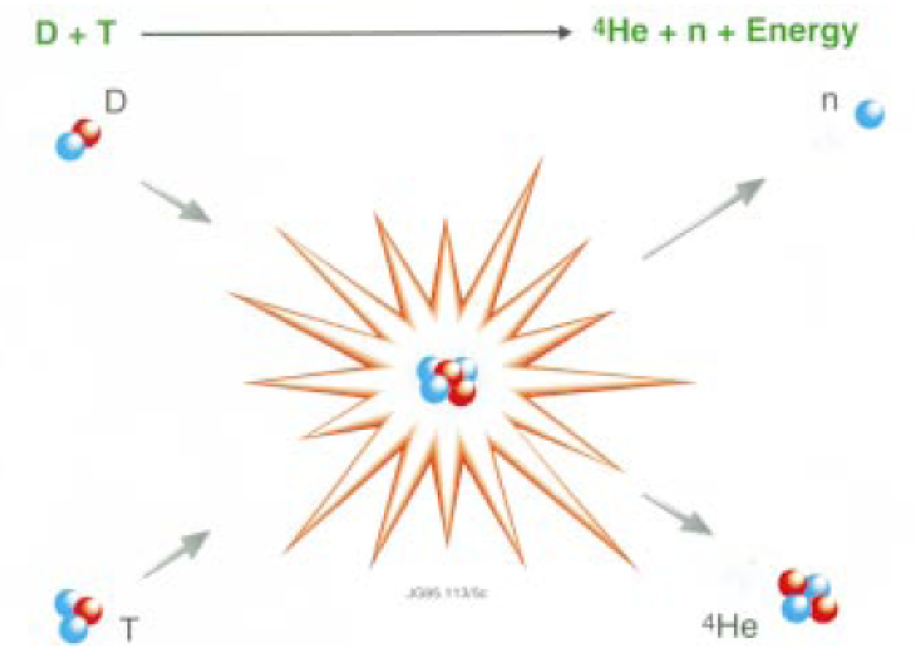
  - Krylov space methods for linear system

Transport equations

■ Atoms	- Rarified Gas Flow
■ Neutral Particles	- Neutrons & Gamma
■ Charged Particles	- Coulomb Interaction
■ Brownian Particles	- Aerosol Physics
■ Thermal-Photons	- Radiative Transfer
■ Electrons & Ions in a Plasma	- Self-consistent Fields

Fusion reactors

Nuclear fusion process



The D-T fusion reaction.

$$D + T \rightarrow He\ (3.5\ MeV) + n\ \ (14.1\ MeV)$$

Fusion of 50:50 mixture of D & T ≈ 80.4 x 10^{12} calories /kg

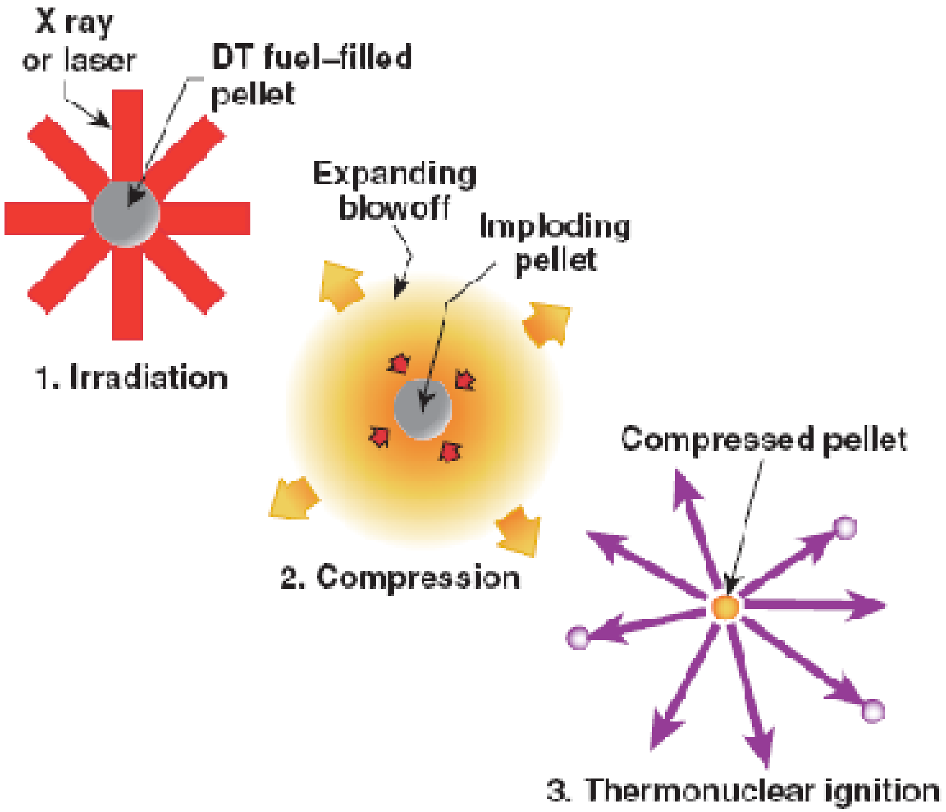
Complete fission of U^{235} generates ≈17.6 x 10^{12} calories /kg

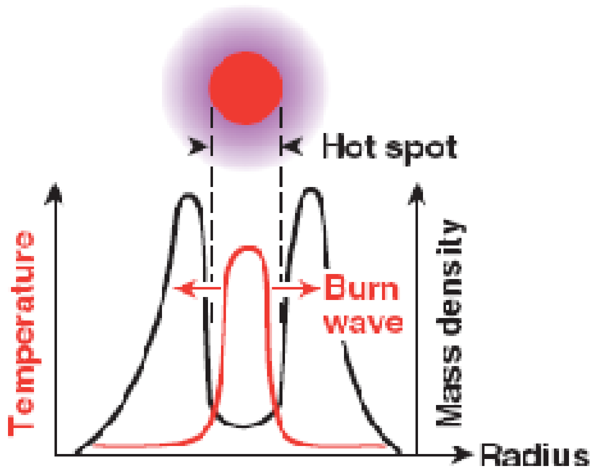
Realizing fusion energy

- Inertial confinement fusion
  - Lasers
  - Ion beams
  - Electron beams

- Magnetic confinement fusion
  - Toroidal systems
  - Open ended systems

Inertial confinement fusion





Time-history of laser pulse is tailored so that a series of multiple shocks generate nearly isentropic compression

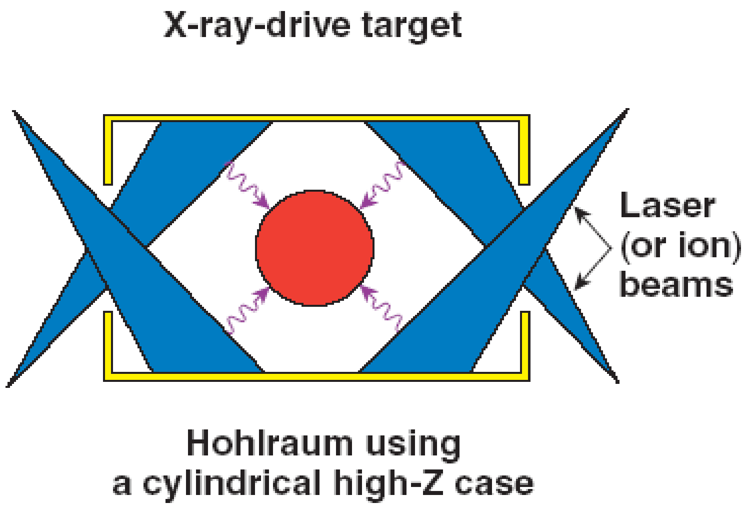
Hot spot parameters for ignition condition:

Temperature ~ 10 keV
Ariel density ~ 0.3 g /cm2

1 keV = 1.16 x 10 ^{7} K

Indirectly driven fusion

- Lasers or ion beams generate x-rays in a hohlraum:



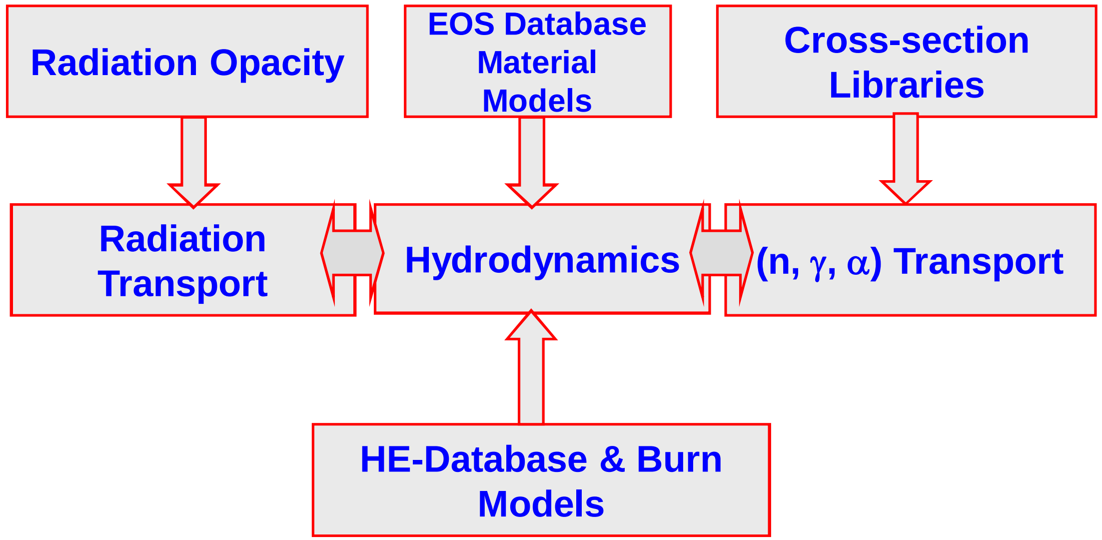
- Laser beams generate X-rays on striking the wall
- X-rays re-distribute inside the gold cylinder
- Capsule is imploded by the uniform X-rays (200 eV)

Several disciplines are involved in simulations

- Material ablation due to x-rays
- Formation of shock waves
- Implosion leads to fusion
- (n, γ, α) transport

- Radiation transport
- Hydrodynamics
- Fusion physics
- transport theory

Need for different databases



A radiation transfer model

- Radiation diffuses through the medium via multiple absorption and emission - $E_\nu(r,t)$ is its energy density

$$\frac{\partial}{\partial t} E_\nu(\vec{r},t) = \nabla \cdot [\frac{c}{3\kappa_\nu} \nabla E_\nu(\vec{r},t)] + c\,\kappa_\nu\,[B_\nu(T) - E_\nu\,]$$

$$\frac{\partial}{\partial t} C_V\,T(\vec{r},t) = \quad c\int_0^\infty \kappa_\nu\,[E_\nu - B_\nu(T)]\,d\nu$$

- Second equation models changes in the temperature of the medium
- Cross-section for absorption $\kappa_\nu(T)$ depends on temperature

- Radiation transfer is generally also coupled to hydrodynamics

Radiation hydrodynamics

RH is the minimal mathematical model for simulating ICF

$$\frac{\partial}{\partial t}\rho + \nabla\cdot(\vec{u}\,\rho) = 0$$

$$\frac{\partial}{\partial t}[\rho\,\vec{u}] + \nabla\cdot[\vec{u}\,\vec{u}\,\rho] + \nabla p = 0$$

$$C_e\frac{\partial T_e}{\partial t} = -[B_e + p_e]\frac{\partial V}{\partial t} + \nabla\cdot[D_e\nabla T_e] + \rho\,C_e\omega_{ie}(T_i - T_e) +$$

$$+\ c\int_0^\infty \kappa_\nu\,[E_\nu - B_\nu(T)]\,d\nu + S_{Fe} + S_L$$

$$C_i\frac{\partial T_i}{\partial t} = [B_i + P_i]\frac{\partial V}{\partial t} + \nabla\cdot[D_i\nabla T_i] - \rho\,C_i\omega_{ie}(T_i - T_e) + S_{Fi}$$

$$\rho\frac{\partial}{\partial t}[E_\nu(\vec{r},t)/\rho] = \nabla\cdot[\frac{c}{3\,\kappa_\nu}E_\nu(\vec{r},t)] + c\,\rho\,\kappa_\nu\,[B_\nu(T) - E_\nu\,] + S_\nu(\vec{r},t)$$

Slowing down of charged particles

- Fusion reactions invariably produce charged particles

$$D + T \rightarrow \alpha\ (3.5\ \text{MeV}) + n\ (14.1\ \text{MeV})$$

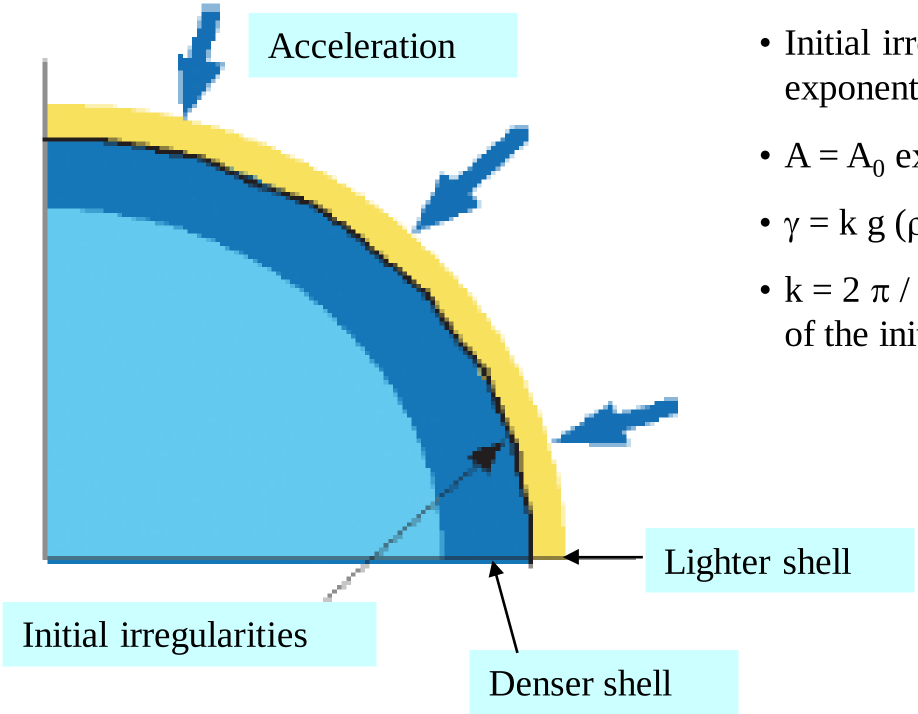
- Energy deposited by charge particles in the plasma
- Transport equation for α-particles

$$\frac{\partial N}{\partial t} + \vec{v} \cdot \nabla_r N + \vec{a} \cdot \nabla_v N = S_\alpha - N\, \nabla_v \cdot \vec{a}$$

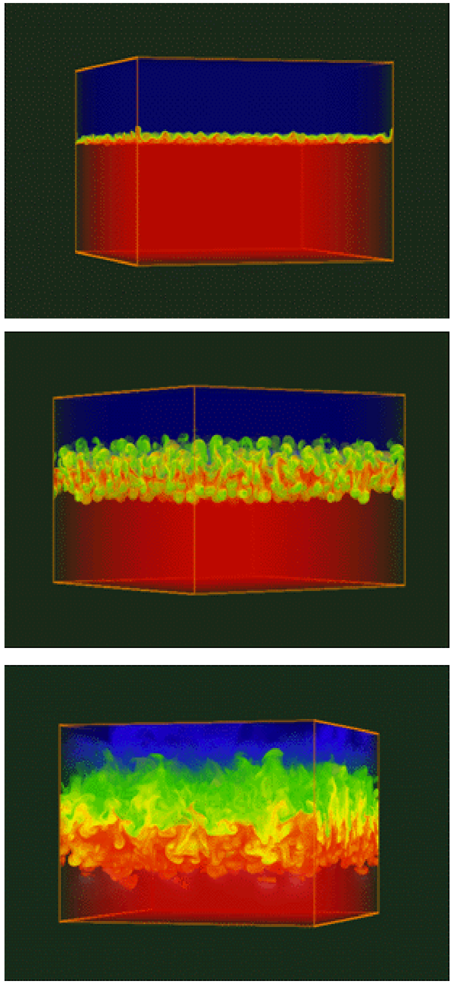
  - Effective acceleration accounts for Coulomb energy loss
- ICF simulations are essentially multi-physics
  - Hydrodynamics
  - Neutron transport
  - Radiation transport
  - Charge particle transport

Rayleigh-Taylor instability

Rayleigh-Taylor instability arises when a light fluid accelerates into a dense fluid

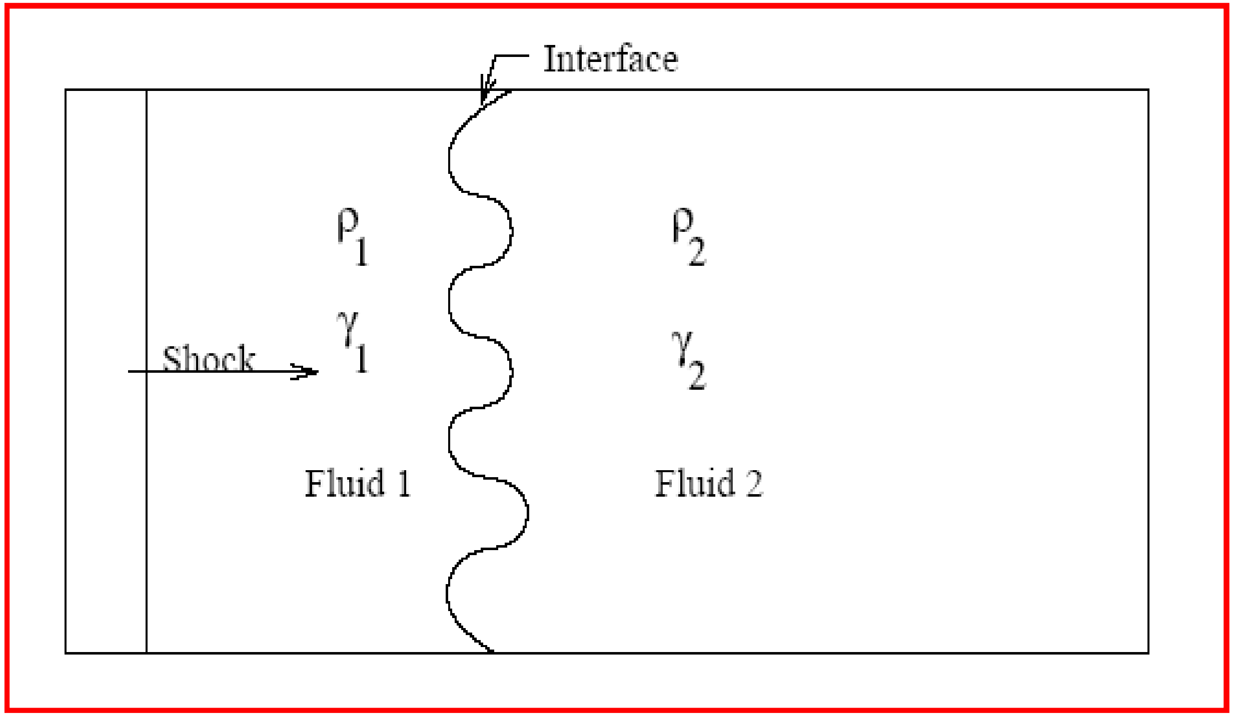


- Initial irregularities grow exponentially in time
- $A = A_0 \exp(\gamma t)$
- $\gamma = k g (\rho_2 - \rho_1) / (\rho2 + \rho1)$
- $k = 2 \pi / \lambda$ wave number of the initial irregularity



3D simulations of development of Raleigh Taylor instability at three different times. Blue is 2 times denser than red

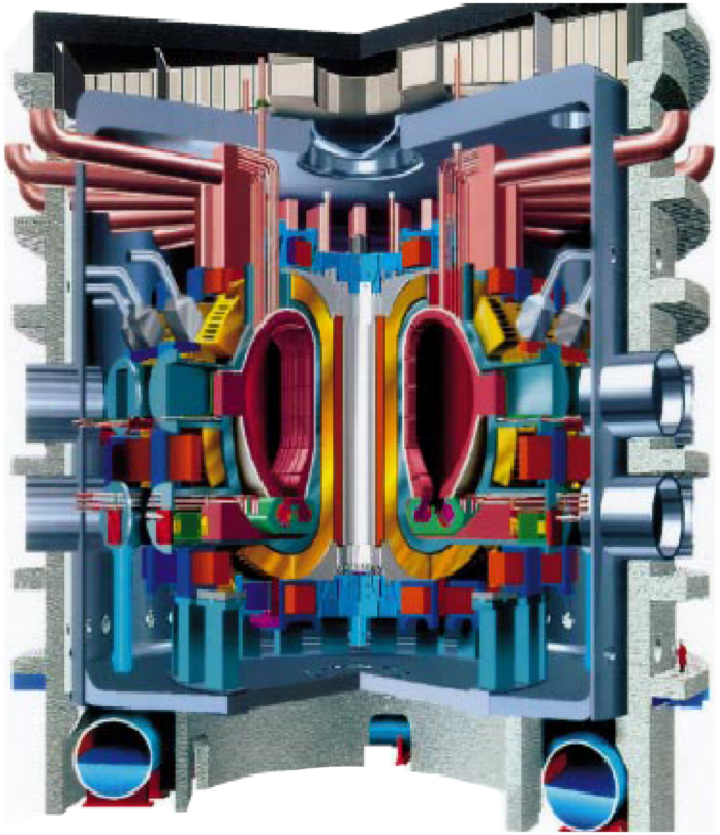
RM instability



- Manufacturing methods produce perturbed interfaces of materials
- Ritchmyer-Meshkov instability arises when a shock wave hits an irregular interface

Magnetic fusion

- In the tokomak chamber, plasma is confined by magnetic fields
  - field along the torous
  - field along the axis
- The plasma moves along the torus
- In-homogeneities and collisions lead to plasma instabilities



Magneto hydrodynamic model

- Plasmas in magnetic confinement fusion is described as double fluids of ions and electrons

$$\frac{\partial n_e}{\partial t} + \nabla \cdot (n_e V_e) = 0 \qquad \frac{\partial n_i}{\partial t} + \nabla \cdot (n_i V_i) = 0$$

$$n_e m_e \frac{\partial V_e}{\partial t} = -\nabla p_e - e n_e (E + V_e \times B) + R \qquad n_i m_i \frac{\partial V_i}{\partial t} = -\nabla p_i + Z e n_i (E + V_i \times B) - R$$

$$\nabla \times E = -\frac{\partial B}{\partial t}$$

$$\frac{1}{\mu_0} \nabla \times B = [-e n_e V_e + Z e n_i V_i] + \frac{\partial D}{\partial t}$$

$$\nabla \cdot D = [-e n_e + Z e n_i]$$

$$\nabla \cdot B = 0$$

Objectives

- Nuclear technology centered around
  - Fission systems
  - Fusion systems
- Design and analysis of the systems
  - Significant amount of mathematical modeling
  - Realistic modeling with fast computers
    - Numerical methods and computing tools
- Feasibility of reducing experiments
- Analysis of laboratory systems
  - Feedback to improved designs
- Operation of nuclear systems

Methods needing attention

- Multi-grid techniques
- Non-orthogonal meshes
- FEM for hydrodynamics
- Preconditioning methods
- Wavelets and applications

Scope for collaborations

- Interaction with expert groups for:
  - Choice of proper algorithms
  - Mathematical base of algorithms
  - Comparative studies

- Numerical schemes for parallel computers
  - Inherently parallel algorithms
  - Error propagation in parallel computations

- Codes for specific problems
  - Study of fluid instabilities
  - Inverse problems