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School on Physics, Technology and Applications of Accelerator Driven Systems (ADS)

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ADS Dynamics "Accelerator-Driven System Dynamics

Part I"

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Accelerator-driven system dynamics

Part I

Politecnico di Torino Dipartimento di Energetica



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Preface

Piero Ravetto:

- Professor of nuclear reactor physics
- Chair of the nuclear and energy engineering program

Activities on reactor physics Transport theory:

- Development of algorithms in $P_{\rm N}$ and $S_{\rm N}$ framework (FEM, BEM ...)
- Treatment of high anisotropy problems and reduction of rayeffects
- Propagation phenomena

Activities on reactor physics Reactor dynamics:

- Development of algorithms and codes (quasi-statics, multipoint...)
- ADS dynamics
- Interpretation of experiments

Activities on reactor physics Innovative reactor technology:

- Models and methods for fluid-fuel (molten-salt) systems
- Liquid-lead cooled reactors

Standard tasks of reactor physics 1.

Describe basic phenomena of neutron motion in material systems: neutronic design of steady-state critical reactors Provide multiplication parameters and flux distributions

Standard tasks of reactor physics 2.

Short scale dynamic simulation

Provide information on transient behaviour in operational and accident conditions for stability and safety assessments

Standard tasks of reactor physics 3.

Long scale dynamic simulation

Provide information on burn-up and nuclide evolution for fuel management

A new challenge of reactor physics

Neutronic design of source-driven systems New features in static and dynamic simulations Need to develop specific models and algorithms

The equation is of deterministic nature, the balance is based on statistical principles The equation for neutrons can be derived from the original non-linear equation for particles in a force field removing the force term and assuming neutron collisions only with a fixed bakground of nuclei (equation becomes linear)

Transport (kinetic) theory plays a fundamental role for all the standard and advanced tasks of reactor physicists



Ludwig E. Boltzmann (1844 - 1906)

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- To write the particle balance probabilities per unit neutron path are needed: cross section $\Sigma(\mathbf{r}, E)$
- Emission function is also needed $f(\mathbf{r}, E' \rightarrow E, \Omega' \cdot \Omega)$
- Note: isotropic medium is supposed (does not imply isotropic emissions - important consideration for ADS!)

[J.J Duderstadt, W. Martin, Transport Theory]

Neutron track length per unit volume, per unit energy, per unit solid angle, per unit time: neutron flux (velocity x density)

 $\varphi(\mathbf{r}, E, \Omega, t)$

Elementary neutron current vector, neutrons crossing the unit oriented area at one space point per unit time, per unit energy, per unit solid angle

 $\Omega \varphi(\mathbf{r}, E, \Omega, t)$

Integro-differential form (first order)

Local balance of particles

$$\frac{1}{v(E)} \frac{\partial \varphi(\mathbf{r}, E, \Omega, t)}{\partial t} + \nabla \cdot \Omega \varphi(\mathbf{r}, E, \Omega, t) + \Sigma(\mathbf{r}, E) \varphi(\mathbf{r}, E, \Omega, t)$$
$$= \int dE' \oint d\Omega' \Sigma(\mathbf{r}, E') \varphi(\mathbf{r}, E', \Omega', t) f(\mathbf{r}, E' \to E, \Omega' \cdot \Omega) + S(\mathbf{r}, E, \Omega, t)$$

 $\varphi(\mathbf{r}, E, \Omega, t = 0) = \varphi_0(\mathbf{r}, E, \Omega)$ Initial conditions

 $\varphi(\mathbf{r}_S, E, \Omega_{in}, t) = 0$ Vacuum boundary conditions

Integro-differential form (second order, isotropic emissions)

even flux $\psi(\mathbf{r}, E, \Omega, t) = \frac{1}{2} \left[\varphi(\mathbf{r}, E, \Omega, t) + \varphi(\mathbf{r}, E, -\Omega, t) \right]$

odd flux $\chi(\mathbf{r}, E, \Omega, t) = \frac{1}{2} \left[\varphi(\mathbf{r}, E, \Omega, t) - \varphi(\mathbf{r}, E, -\Omega, t) \right]$

Integral form

Global balance of particles

 $\varphi({\bf r},E,\Omega,t) =$

$$= \int_{0}^{Min[s_{0}(\mathbf{r},\Omega),vt]} ds \left[\int dE' \oint d\Omega' \Sigma(\mathbf{r} - s\Omega, E') \varphi(\mathbf{r} - s\Omega, E', \Omega', t - \frac{s}{v}) f(\mathbf{r} - s\Omega, E' \to E, \Omega' \cdot \Omega) \right. \\ \left. + S(\mathbf{r} - s\Omega, E, \Omega, t - \frac{s}{v}) \right] \exp\left(- \int_{0}^{s} ds' \Sigma(\mathbf{r} - s'\Omega, E) \right)$$

Integral form for isotropic emissions: Peierls equation

$$\begin{split} \Phi(\mathbf{r}, E, t) &= \frac{1}{4\pi} \int d\mathbf{r}' \left[\int dE' \oint d\Omega' \Sigma(\mathbf{r}', E') \Phi(\mathbf{r}', E', t - \frac{|\mathbf{r} - \mathbf{r}'|}{v}) f(\mathbf{r}', E' \to E) \right. \\ &+ \left. S(\mathbf{r}', E, t - \frac{|\mathbf{r} - \mathbf{r}'|}{v}) \right] \frac{\exp\left(- \int_{0}^{|\mathbf{r} - \mathbf{r}'|} ds' \Sigma(\mathbf{r} - s'\Omega, E) \right)}{|\mathbf{r} - \mathbf{r}'|^2} \end{split}$$

The Monte Carlo approach

The full statistical simulation retrieves information on the solution of the integral equation The simulation is performed on the basis of elementary interaction probability laws

The emission from fission

$$\begin{split} &\frac{1}{v(E)} \frac{\partial \varphi(\mathbf{r}, E, \Omega, t)}{\partial t} + \nabla \cdot \Omega \varphi(\mathbf{r}, E, \Omega, t) + \Sigma(\mathbf{r}, E) \varphi(\mathbf{r}, E, \Omega, t) \\ &= \int dE' \oint d\Omega' \Sigma_s(\mathbf{r}, E') \varphi(\mathbf{r}, E', \Omega', t) f_s(\mathbf{r}, E' \to E, \Omega' \cdot \Omega) \\ &+ \frac{\chi(\mathbf{r}, E)}{4\pi} \int dE' \Sigma_f(\mathbf{r}, E') \oint d\Omega' \varphi(\mathbf{r}, E', \Omega', t) + S(\mathbf{r}, E, \Omega, t) \end{split}$$

The emission from fission: delayed neutrons

$$\begin{split} &\frac{1}{v(E)} \frac{\partial \varphi(\mathbf{r}, E, \Omega, t)}{\partial t} + \nabla \cdot \Omega \varphi(\mathbf{r}, E, \Omega, t) + \Sigma(\mathbf{r}, E) \varphi(\mathbf{r}, E, \Omega, t) \\ &= \int dE' \oint d\Omega' \Sigma_s(\mathbf{r}, E') \varphi(\mathbf{r}, E', \Omega', t) f_s(\mathbf{r}, E' \to E, \Omega' \cdot \Omega) \\ &+ \frac{\chi(\mathbf{r}, E)}{4\pi} \left(1 - \beta\right) \int dE' \Sigma_f(\mathbf{r}, E') \oint d\Omega' \varphi(\mathbf{r}, E', \Omega', t) \\ &+ \sum_{i=1}^R \lambda_i G(\mathbf{r}, t) \frac{\chi_i(\mathbf{r}, E)}{4\pi} + S(\mathbf{r}, E, \Omega, t) \end{split}$$

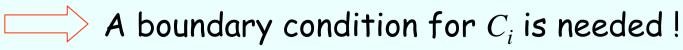
The emission from fission: delayed neutrons

Additional equations are needed for delayed precursors For solid fuel:

$$\frac{\partial C_{i}(\mathbf{r},t)}{\partial t} = \beta_{i} \int dE' \nu \Sigma_{f}(\mathbf{r},E') \oint d\Omega' \varphi(\mathbf{r},E',\Omega',t) - \lambda_{i} C_{i}(\mathbf{r},t)$$

For fluid fuel:

$$\frac{\partial C_{i}(\mathbf{r},t)}{\partial t} = \beta_{i} \int dE' \nu \Sigma_{f}(\mathbf{r},E') \oint d\Omega' \varphi(\mathbf{r},E',\Omega',t) - \lambda_{i} C_{i}(\mathbf{r},t) - \nabla \cdot [\mathbf{V}(\mathbf{r},t)C_{i}(\mathbf{r},t)]$$



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"Simple" transport models

Steady-state monokinetic equation in plane geometry, isotropic emissions

Integro-
Differential
$$\mu \frac{\partial \varphi(x,\mu)}{\partial x} + \Sigma \varphi(x,\mu) = \frac{\Sigma_s}{2} \int_{-1}^{1} d\mu' \varphi(x,\mu') + \frac{1}{2} S(x)$$

Integral
$$\Phi(x) = \frac{1}{2} \int dx' E_1 \left(\Sigma |x - x'| \right) \left[\Sigma_s \Phi(x') + S(x') \right]$$

However "simple" ... it constitutes a tremendous physico-mathematical task ...

$$\begin{aligned} &\frac{1}{v(E)} \frac{\partial \varphi(\mathbf{r}, E, \Omega, t)}{\partial t} + \nabla \cdot \Omega \varphi(\mathbf{r}, E, \Omega, t) + \Sigma(\mathbf{r}, E) \varphi(\mathbf{r}, E, \Omega, t) \\ &= \int dE' \oint d\Omega' \Sigma(\mathbf{r}, E') \varphi(\mathbf{r}, E', \Omega', t) f(\mathbf{r}, E' \to E, \Omega' \cdot \Omega) + S(\mathbf{r}, E, \Omega, t) \end{aligned}$$

$$\nabla \cdot \Omega \varphi(\mathbf{r}, E, \Omega) + \Sigma(\mathbf{r}, E) \varphi(\mathbf{r}, E, \Omega)$$

= $\int dE' \oint d\Omega' \Sigma_s(\mathbf{r}, E') \varphi(\mathbf{r}, E', \Omega') f_s(\mathbf{r}, E' \to E, \Omega' \cdot \Omega)$
+ $\frac{\chi(\mathbf{r}, E)}{4\pi} \int dE' \nu \Sigma_f(\mathbf{r}, E') \oint d\Omega' \varphi(\mathbf{r}, E', \Omega') + S(\mathbf{r}, E, \Omega)$

$$\nabla \cdot \Omega \varphi(\mathbf{r}, E, \Omega) + \Sigma(\mathbf{r}, E) \varphi(\mathbf{r}, E, \Omega)$$

$$= \int dE' \oint d\Omega' \Sigma_s(\mathbf{r}, E') \varphi(\mathbf{r}, E', \Omega') f_s(\mathbf{r}, E' \to E, \Omega' \cdot \Omega)$$

$$+ \frac{\chi(\mathbf{r}, E)}{4\pi} \int dE' \nu \Sigma_f(\mathbf{r}, E') \oint d\Omega' \varphi(\mathbf{r}, E', \Omega')$$

$$\nabla \cdot \Omega \varphi(\mathbf{r}, E, \Omega) + \Sigma(\mathbf{r}, E) \varphi(\mathbf{r}, E, \Omega)$$

$$= \int dE' \oint d\Omega' \Sigma_s(\mathbf{r}, E') \varphi(\mathbf{r}, E', \Omega') f_s(\mathbf{r}, E' \to E, \Omega' \cdot \Omega)$$

$$+ \left[\frac{1}{k}\right] \frac{\chi(\mathbf{r}, E)}{4\pi} \int dE' \nu \Sigma_f(\mathbf{r}, E') \oint d\Omega' \varphi(\mathbf{r}, E', \Omega')$$

$$\nabla \cdot \Omega \varphi(\mathbf{r}, E, \Omega) + \Sigma(\mathbf{r}, E) \varphi(\mathbf{r}, E, \Omega)$$

$$= \left[\frac{1}{\gamma} \right] \left[\int dE' \oint d\Omega' \Sigma_{s}(\mathbf{r}, E') \varphi(\mathbf{r}, E', \Omega') f_{s}(\mathbf{r}, E' \to E, \Omega' \cdot \Omega) \right]$$

$$+ \frac{\chi(\mathbf{r}, E)}{4\pi} \int dE' \nu \Sigma_{f}(\mathbf{r}, E') \oint d\Omega' \varphi(\mathbf{r}, E', \Omega') \right]$$

$$\nabla \cdot \Omega \varphi(\mathbf{r}, E, \Omega) + \left[\Sigma(\mathbf{r}, E) + \frac{\alpha}{v} \right] \varphi(\mathbf{r}, E, \Omega)$$

$$= \int dE' \oint d\Omega' \Sigma_{s}(\mathbf{r}, E') \varphi(\mathbf{r}, E', \Omega') f_{s}(\mathbf{r}, E' \to E, \Omega' \cdot \Omega)$$

$$+ \frac{\chi(\mathbf{r}, E)}{4\pi} \int dE' \nu \Sigma_{f}(\mathbf{r}, E') \oint d\Omega' \varphi(\mathbf{r}, E', \Omega')$$

$$\nabla \cdot \frac{\Omega \varphi(\mathbf{r}, E, \Omega)}{\left[\int dE' \oint d\Omega' \Sigma_{s}(\mathbf{r}, E') \varphi(\mathbf{r}, E', \Omega') f_{s}(\mathbf{r}, E' \to E, \Omega' \cdot \Omega) + \frac{\chi(\mathbf{r}, E)}{4\pi} \int dE' \nu \Sigma_{f}(\mathbf{r}, E') \oint d\Omega' \varphi(\mathbf{r}, E', \Omega') - \Sigma(\mathbf{r}, E) \varphi(\mathbf{r}, E, \Omega)\right]$$

Eigenvalue: various formulations

Multiplication k Collision γ Time α Density δ

Eigenvalue

The time eigenvalue can be defined to include delayed neutron information (w-modes)

$$\begin{split} &\nabla \cdot \Omega \varphi(\mathbf{r}, E, \Omega) + \left[\Sigma(\mathbf{r}, E) + \left(\frac{\alpha}{v} \right) \varphi(\mathbf{r}, E, \Omega) \right. \\ &= \int dE' \oint d\Omega' \Sigma_{s}(\mathbf{r}, E') \varphi(\mathbf{r}, E', \Omega') f_{s}(\mathbf{r}, E' \to E, \Omega' \cdot \Omega) \\ &+ \frac{1}{4\pi} \left[(1 - \beta) \chi_{p}(\mathbf{r}, E) + \sum_{i=1}^{R} \left(\frac{\beta_{i}}{\alpha + \lambda_{i}} \chi_{i}(\mathbf{r}, E) \right] \int dE' \nu \Sigma_{f}(\mathbf{r}, E') \oint d\Omega' \varphi(\mathbf{r}, E', \Omega') \right] \\ \end{split}$$

What is a critical system?

A system for which a non-zero solution exists in the absence of any external source !

Hence: k=1 a=0

What is a subcritical system?

A system for which fission production cannot compensate losses due to streaming (leakage through the boundary) and net removal through collisions; only by a source a steady-state can be established !

Hence: k<1

α<0

What is a supercritical system?

A system for which fission production is larger than losses due to streaming (leakage through the boundary) and net removal through collisions; no steady-state can be established !

Hence: k>1 a>0

A digression on analytical methods

Why analytical methods?

- To grasp the mathematical nature of the problem
- To get full insight into physics
- To obtain reference solutions

The analysis of the transport problem in the Fourier-transformed space

[Case, DeHoffmann, Placzek, Introduction to the Theory of Neutron Diffusion]

$$\tilde{\Phi} = \frac{\frac{1}{B} \arctan \frac{B}{\Sigma}}{1 - c\Sigma \frac{1}{B} \arctan \frac{B}{\Sigma}} \tilde{S}(B) \equiv \Gamma(B) \tilde{S}(B)$$

Frequency analysis of the problem

The analysis of the transport problem in the Fourier-transformed space

All approximations to the transport model amount to a suitable approximation of the transport kernel

$$\mathbf{S}_{\mathsf{N}} \qquad \Gamma(B) \simeq \frac{\frac{1}{2} \sum_{n=1}^{N} \frac{w_n}{iB\mu_n + \Sigma}}{1 - \frac{c\Sigma}{2} \sum_{n=1}^{N} \frac{w_n}{iB\mu_n + \Sigma}} = \frac{\sum_{n=1}^{N/2} \frac{w_n\Sigma}{B^2\mu_n^2 + \Sigma^2}}{1 - c\Sigma \sum_{n=1}^{N/2} \frac{w_n\Sigma}{B^2\mu_n^2 + \Sigma^2}}$$

diffusion
$$\Gamma(B) \simeq \frac{1}{\frac{\tilde{\mu}^2}{\Sigma}B^2 + \Sigma(1-c)} \left[= \frac{1}{\frac{1}{3\Sigma}B^2 + \Sigma_a} \right]$$

The analysis of the transport problem in the Fourier-transformed space

$$\Gamma(B) \simeq \frac{\frac{1}{\xi(B)} \arctan \frac{\xi(B)}{\Sigma}}{1 - c\Sigma \frac{1}{\xi(B)} \arctan \frac{\xi(B)}{\Sigma}}$$

Space discretization

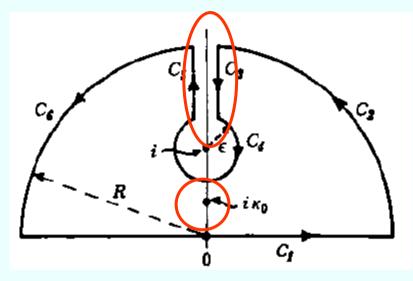
$$\xi(B) = \frac{\sin\left(B\frac{\Delta x}{2}\right)}{\frac{\Delta x}{2}}$$

The Fourier transform can be inverted

- Fundamental work by Case-DeHoffmann-Placzek
- It is possible to obtain the exact Green function of the problem
- The Fourier transform is characterized by a polar singularity and a branch-cut (discrete and continuous spectra)
- The residue in the pole yields a diffusion-like contribution
- The integral along the branch-cut yields the "typical" transport behaviour

Singularities





The poles characterize the spatial relaxation length of the asymptotic portion of the solution, the branch cut describes the "transient" behaviour

The Fourier transform can be inverted

Fully analytical solution:

$$\Phi_{exact}(r) = K \frac{e^{-r/L}}{r} + \frac{1}{r} \int_{\Sigma}^{+\infty} dy F(y) e^{-ry}$$

$$\equiv \Phi_{diffusion}(r) + \Phi_{transport}(r) \equiv \Phi_{pole}(r) + \Phi_{branch-cut}(r)$$

$$\equiv \Phi_{asymptotic}(r) + \Phi_{transient}(r)$$

Case method

[K.M. Case, P.F. Zweifel, *Linear Transport Theory*] Method of singular eigenfunctions: The solution to the transport equation is "expanded" as a sum of a term containing the discrete eigenfunctions and an integral term (!), containing the superposition of continuous eigenfunctions

Case method

$$\Phi_{exact}(x,\mu) = A_{+}\psi_{0}^{+}(\mu)e^{-x/\nu_{0}} + A_{-}\psi_{0}^{-}(\mu)e^{x/\nu_{0}} + \int_{-1}^{1} d\nu A(\nu)\psi_{\nu}(\mu)e^{-x/\nu}$$
Asymptotic solution
"Transport" solution

Solution of the transport problem for realistic configurations

The usual "engineering" procedure for too complicated deterministic physicomathematical problems:

- 1. Approximate the model (physics is distorted), e.g. transport \rightarrow diffusion
- 2. Solve equations of approximate model by algorithms (numerically induced effects are introduced ... discretizations, truncations ... further distortions of physics)

Solution of the transport problem for realistic configurations

The Monte Carlo method avoids physical distortions of 1. and 2.

however

Statistical uncertainties are introduced

Basics of reactor calculations

Split the full problem (too complicate) into a succession of problems trying to separate specific aspects and treat them separately (multi-scale) Well-known technique in engineering

Basics of reactor calculations: dynamics

Handle numerical stiffness Reduce the complication of the full problem

1. Spherical harmonics [B. Davison, *Transport Theory*]

Idea:

To expand angular dependence as a truncated series of spherical harmonics functions

1. Spherical harmonics

Solve a space-energy integrodifferential system for the expansion coefficients (angular moments)

1. Spherical harmonics

Advantages

- no angular distorsion
- coupling of nearest moments only
- good mathematical and physical properties of the method
- low-order: diffusion

1. Spherical harmonics Example: plane geometry with anisotropic scattering

$$\Phi(x,\mu,t) = \sum_{n=0}^{\infty} \frac{2n+1}{2} \Phi_n(x,t) P_n(\mu)$$

$$S(x,\mu,t) = \sum_{n=0}^{\infty} \frac{2n+1}{2} S_n(x,t) P_n(\mu)$$

1. Spherical harmonics Physical meaning of first moments

$$\Phi(x,t) = \int_{-1}^{1} d\mu \Phi(x,\mu,t) = \Phi_0(x,t)$$
 Total flux

$$J(x,t) = \int_{-1}^{1} d\mu \mu \Phi(x,\mu,t) = \Phi_1(x,t)$$
 Total current

1. Spherical harmonics

Expansion of scattering cross section:

$$\oint d\Omega' \sum_{n=0}^{\infty} \frac{2n+1}{2} \Sigma_n(x) P_n(\Omega \cdot \Omega') \Phi(x, \mu', t) = \sum_{n=0}^{\infty} \frac{2n+1}{2} \Sigma_n(x) \Phi_n(x, t) P_n(\mu)$$

General equation:
$$-\frac{1}{v}\frac{\partial \Phi_{n}(x,t)}{\partial t} - \Sigma \Phi_{n}(x,t) + \Sigma_{n} \Phi_{n}(x,t) + S_{n}(x,t)$$

$$=\frac{n+1}{2n+1}\frac{\partial \Phi_{n+1}(x,t)}{\partial t}+\frac{n}{2n+1}\frac{\partial \Phi_{n-1}(x,t)}{\partial t}$$

1. Spherical harmonics **Disadvantages**

- complication and large number of equations in multi-D
- complicate numerical methods are needed for space discretization of first-order operators

2. Discrete ordinates [based on method of Wick Chandrasekhar]

Idea:

To discretize the direction unit vector and to use a proper integration formula for collision terms

2. Discrete ordinates

Solve a space energy system for direction fluxes

2. Discrete ordinates

Example: plane geometry with anisotropic scattering

$$\frac{1}{v}\frac{\partial \Phi(x,\mu_{i},t)}{\partial t} + \mu_{i}\frac{\partial \Phi(x,\mu_{i},t)}{\partial \mu} - \Sigma \Phi(x,\mu_{i},t) = \sum_{j=0}^{N} \Sigma_{ij}\Phi(x,\mu_{j},t) + S(x,\mu_{i},t)$$

Angular transfer cross-section:

$$\Sigma_{ij} = \sum_{n=0}^{L} \frac{2n+1}{2} \Sigma_n w_j P_n(\mu_i) P_n(\mu_j)$$

- 2. Discrete ordinates Advantages
- simple derivation of the method
- unknowns retain physical meaning

- 2. Discrete ordinates
- Disadvantages
- full coupling of unknowns
- balance equations are not sufficient to close the equations; need of transmission relations
- complications in multi-D
- ray effect distorsions for time dependent and multi-D problems

3. Collision probabilities

Idea:

Subdivide the spatial domain into subdomains and use the integral equation to generate a system describing the integral balance through spatial coupling among subdomains

- 2. Collision probabilities Advantages
- simple derivation and numerical stability
- physically meaningful
- no ray effect

2. Collision probabilities Disadvantages

- limitation to isotropic or linearlyanisotropic scattering
- complicate calculation of spatial integrals in multi-D

The solution of the transport equation: New challenges

- Use better angular descriptions (angular finite elements, characteristics, boundary elements)
- 1. Remove ray effects (e.g., source-driven problems)
- 2. Treat complicated configurations
- 3. Treat high streaming systems (e.g., fusion blankets)

Hope: not to change the physico-mathematical structure of the problem ...)

The solution of the transport equation: New challenges

Improve the representation of scattering

- 1. High anisotropy scattering problems (high energy source problems)
- 2. Shortcoming of Legendre representation of scattering function (either unphysical behaviour or high order expansion)
- 3. Radiative transfer problems

The solution of the transport equation: tools to meet new challenges

- 1. Method of characteristics
- 2. Simplified spherical harmonics and A_N
- 3. Second-order and angular finite elements
- 4. Nodal and response matrix formulation
- 5. Boundary element techniques
- 6. Domain decomposition, coupling of statistical and deterministic techniques
- 7. Stochastic transport