ICTT 2022

27th International Conference on Transport Theory

Bertinoro (Forlì, Italy), 10-16 July 2022

Book of abstracts

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ICTT-27 SCIENTIFIC PROGRAM

MONDAY 11/07		
9.30		***Welcome address***
10.00	B.D. Ganapol	***Introduction to ICTT-27***
11.00	Vincenzo Molinari (D. Giusti)	***On the statistical model of the atom***
11.25	Vincenzo Molinari (D. Mostacci)	***Kinetic theory study of pressure and EoS in a strongly degenerate Fermi gas***
11.50		***Coffee break***
12.10	Laura Laghi	***Physics-Informed Neural Networks for Linear One-Dimensional Diffusion-Advection-Reaction Equations***
12.35	Jean C. Ragusa	***Physics-informed Neural Network with Fourier Features for Radiation Transport in Heterogeneous Media***
13.00	Enrico Schiassi	***Physics-Informed Neural Networks for the Point Kinetics Equations for Nuclear Reactor Dynamics***
13.25		***Lunch***
15.00	B.D. Ganapol	***Response Matrix Discrete Ordinates Solution of the 1D Fokker-Planck Equation***
15.25	A. Previti	***Towards a systematic requirement based approach to build a neutronic study platform***
15.50	David Labeurthre	***About the construction of finite element bases on 3D hexagonal geometries for neutron transport simulation***
16.15		***Coffee break***
16.35	Dmitriy Anistratov	***Analysis of Noise Effects in Hybrid Transport Methods Based on Low-Order Moment Equations***
17.00	Farzad Rahnema	***A Hybrid High-Order Low-Order COMET Method for Solving Eigenvalue Neutron Transport Problems***
17.25	Johan Cufe	***On the accuracy of the Ronen Method in plane geometry***
17.50	Daniele Scannandrone	***A Novel Angular Discretization method for the Neutron Transport Equation: the MPN method***
18.15		***Day closes***

ICTT-27 SCIENTIFIC PROGRAM

TUESDAY 12/07		
9.30	Richard Sanchez (keynote)	***Analysis of the time spectrum of the kinetic transport operator***
10.15	B.D. Ganapol	***Numerical Caseology by Lagrange Interpolation for The 1D Neutron Transport Equation In A Slab***
10.40	M. Tiberga	***A Novel High-Order Surface Characteristics Scheme for the Neutron Transport Equation on 2D Unstructured Meshes***
11.05	P. Saracco	***Benchmarking one group neutron transport equation eigenvalues***
11;30		***Coffee break***
11.50	Ph. Humbert	***Neutron Count Probability Approximations Using Moments, Meixner Polynomial Expansion and N-Forked Approximation***
12.15	T. Keßler	***Entropy-stable Galerkin methods for the Boltzmann equation***
12.40	W. Bennett	***Benchmark Quality Time-dependent Transport Solutions Using a Moving Mesh***
13.05		***Lunch***
15.00	E. Masiello	***Angular flux asymptotic expansion applied to discrete-ordinates source iterations for lattice depletion calculations***
15.25	T. Bonnet	***Analysis of the correlation functions for the neutron and precursor populations at criticality***
15.50	Francesco Filiciotto	***Non-Conforming 3D Model for PWR Control-Rod Movements without Homogenization and Cusping Effect***
16.15	A. Previti	***Comparative analysis between fuel assembly calculation capabilities using APOLLO2 and APOLLO3® codes***
16.40		***Coffee break***
17.00	A. Carpio	***Kinetic models for angiogenesis: analysis and simulation***
17.25	Gael Poette	***Revisiting the learning process in Machine Learning from a partial differential equation point of view: what transport can bring***
17.50	L. L. Bonilla	***Swarm formation***
18.15		***Day closes***

ICTT-27 SCIENTIFIC PROGRAM

THURSDAY 14/07		
9.00	Mario Marengo (keynote)	***State of the art in cyclotrons for radionuclide production in biomedicine***
9.45	Maha Farasat	***Efficiency calibration of a stable NaI(Tl) detector for 41Ar for air exhaust systems***
10.10	Jorge E. Fernandez	***Full Recovering of an X-ray Spectrum from Detector Influence***
10.35	Gael Poette	***Building and solving efficient reduced models for the uncertain linear Boltzman equation: applications to neutronics (keff) and photonics***
11.00	A. Christensen	***First-Collision Source Treatment for Ray Effect Mitigation in Discrete-Ordinate Radiation Transport Solutions***
11.25		***Coffee break***
11.45	Shay I. Heizler	***Discrete implicit Monte-Carlo (DIMC) scheme for simulating radiative transfer problems***
12.10	Richard Vega	***Implicit Monte Carlo with High Order Finite Element Spatial Discretization***
12.35	P. Cosgrove	***Implementation of the Random Ray Method in the Monte Carlo codes SCONE and OpenMC***
13.00	J. Bartsch	***A Monte Carlo framework for optimal control problems governed by multi-species plasma models***
13.25		***Lunch***
15.00	Martina Conte	***Multi-cue kinetic model for cell migration on a fiber network***
15.25	Nadia Loy	***Direction-Dependent Turning Leads to Anisotropic Diffusion and Persistence***
15.50	Y. El-Khatib	***On a regime-switching stochastic epidemic model for COVID-19***
!6:15	D. Laghi	***A new V&V philosophy for fusion nuclear data libraries***
16.40	Vladimir V. Aristov	***Mathematical Simulation of the Spatial Spread of COVID-19 Waves***
17.05		***Day closes***

ICTT-27 SCIENTIFIC PROGRAM

FRIDAY 15/07		
9.00	Eugene d'Eon (keynote)	***Step Correlations in Non-Classical Transport using 1D Point Processes***
10.00	Maria Groppi	***A mixed BGK-Boltzmann model for inert gas mixtures***
10.25	M. Bisi	***A general kinetic model of Boltzmann type for polyatomic gases***
10.50	F. Brini	***A Rational Extended Thermodynamics description of acceleration waves and oscillating gas bubbles***
11.15		***Coffee break***
11.35	V. Romano	***Charge transport in graphene nanoribbons by means of the semiclassical Boltzmann equation***
12.00	G. Vitanza	***Wigner equations for charge and phonons transport in graphene***
12.25	M. Trovato	***The Maximum entropy Principle in solid state physics: General approach for dynamic high-Field transport in semiconductor materials and graphene***
12.50	V.D. Camiola	***A bipolar hydrodynamical model for charge transport in graphene nanoribbons***
13.15	V. Romano	***Equilibrium Wigner function for fermions and bosons and quantum hydrodynamical models for charge transport in graphene***
13.40		***Lunch***
15.30		***ICTT meeting and closing ceremony***

Analysis of Noise Effects in Hybrid Transport Methods Based on Low-Order Moment Equations

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Abstract

Hybrid stochastic/deterministic techniques have been developed for solving particle transport problems. These numerical algorithms use advantages of deterministic methods in generation of the global solution over the phase-space domain to provide Monte Carlo (MC) methods with valuable data for improving computational performance. The hybrid methods involve low-order problems for the moments of the angular flux formulated with data computed in MC cycles. The low-order problem is coupled with MC. This approach has been applied to develop hybrid techniques for reactor-physics and deep-penetration problems [1-3]. Statistical noise influences performance of hybrid schemes in various ways [4].

In this study, we analyse noise phenomena in a two-level hybrid numerical method in which (i) the transport equation is solved with MC and (ii) deterministic moment equations are formulated by the low-order quasidiffusion (aka VEF) equations for the scalar flux and current [5,6]. The problems at two levels are nonlinearly coupled by means of an exact closure defined by the Eddington factor. To analyse noise effects on the solution, we use the system of deterministic equations defined by the discretized transport and low-order equations and solved with fixed point iterations. To model stochastic fluctuations in the MC solution the noise is added to the deterministic solution of the transport equation on every iteration. We study propagation of noise through the system of coupled high-order and low-order equations.

The time-dependent one-group problems in 1D slab geometry are considered. The equations are discretized with the backward Euler time integration method. The transport equation is approximated by the step characteristics. The low-order equations are discretized by the finite volume (FV) scheme. The grid function of the Eddington factor in the FV scheme is its cell-average value. The added noise has the normal distribution with some given variance σ^2 and spatial correlation. A set of numerical results is obtained for different values of σ and spatial correlation lengths. In considered cases, it is observed that the relative error due to added noise is bounded by the standard deviation σ of the noise function.

This work has been funded by Advanced Simulation and Computing Predictive Science Academic Alliance Program (PSAAP III) of US DOE NNSA.

References

1. E. Larsen, J. Yang, A functional Monte Carlo method for k-eigenvalue problems, Nuclear Science and Engineering, **159**, 107-126 (2008).
2. M. Lee, H. Joo, D. Lee, K. Smith, Coarse mesh finite difference formulation for accelerated Monte Carlo eigenvalue calculation, Annals of Nuclear Energy, **65**, 101-113 (2014).
3. T. Becker, A. Wollaber, and E. Larsen, A hybrid Monte Carlo–deterministic method for global particle transport calculations, Nuclear Science and Engineering, **155**, 155-167 (2007).
4. A. Prinja, Effect of spatio-temporal noise in the Eddington factor on the scalar flux, Annals of Nuclear Energy, **86**, 116-122 (2015).
5. V. Gol'din, A quasi-diffusion method of solving the kinetic equation, USSR Computational Mathematics and Mathematical Physics, **4**, 136-149 (1964).
6. L. Auer, D. Mihalas, On the use of variable Eddington factors in non-LTE stellar atmospheres computations, Monthly Notices of the Royal Astronomical Society, **149**, 65-74 (1970).

Mathematical Simulation of the Spatial Spread of COVID-19 Waves

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Abstract

A two-parameter kinetic equation model proposed in [1] is used to describe the spatial spread of the virus through countries in the COVID-19 pandemic. The migration of infection carriers from certain foci inherent in some countries is considered. Different models can describe the evolution of an epidemic in time, for example SIR [2]. The main difference of our model from popular SIR-like models is that it describes the spatial spread of the epidemic (which SIR models do not) when infections inside cities can be neglected. We study the movement of the wave of infections along the selected direction, but we do not consider the entire time evolution of the epidemic in a given area, since a few weeks after the first infections, it is already determined by local infections. The one-dimensional model is applied to three countries: Russia, Italy, and Chile. Both their geographical location and their particular shape stretching in the direction from the centres of infection (Moscow, Lombardy, and Santiago, respectively) make it possible to use such an approximation. Also a two-dimensional model is studied and applied to Russia. Two parameters of the model are derived from known data. The first is the value of the average spreading rate associated with the transfer of infected persons in transport vehicles. Since different means of transport inherently have different travel speeds and the model requires a single velocity value, the least squares method is applied to the data points of first infections in different regions which allows to make a realistic estimation of the spreading rate. The second parameter is the frequency of the decrease in numbers of the infected as they move around the country, associated with the arrival of passengers at their destination and possibly with quarantine measures. An analytical solution is obtained for the one-dimensional case and a numerical solution for the two-dimensional case. Simple numerical methods are also used to perform a series of calculations to make some predictions with the help of the one-dimensional model, for example, a prediction about the time of recovery in Russia, if the beginning of recovery in Moscow is known. The quality of predictions is tested with the help of new data obtained during the second and third waves. Also a prediction for the fourth wave in Russia is made. The forecasts are correct due to the estimated speed of the average traffic and are approximately equal to 3 weeks of delay between the maximum of infections per day in Moscow and Russia.

[1] Aristov VV, Stroganov AV, Yastrebov AD. Simulation of Spatial Spread of the COVID-19 Pandemic on the Basis of the Kinetic-Advection Model. Physics. 2021; 3(1):85-102. https://doi.org/10.3390/physics3010008
[2] Kermack, W.O.; McKendrick, A.G. A contribution to the mathematical theory of epidemics. Proc. R. Soc. Lond. A 1927, 115, 700–721.

A Monte Carlo framework for optimal control problems governed by multi-species plasma models

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Abstract

Kinetic models are used to describe the behaviour of various physical systems on particle level, in particular plasma as it is used in fusion reactors. Much effort has been put in the simulation of such models, but less is known about related problems concerning the calibration and control of such systems. This work is devoted to the theoretical and numerical investigation of ensemble optimal control problems governed by multispecies plasma models. Using an expectation value formulation of the objective and the Lagrange framework for optimal control, it is intended to derive an adjoint plasma model and reformulate it such that it can be interpreted in a kinetic way.
Hence, it is then possible to develop a numerical strategy to solve the plasma model and its adjoint that is consistent with the kinetic description of gas. This is of particular interest, as in certain cases such strategies must be used to solve plasma models in order to avoid inaccuracies that can occur in numerical methods based on continuum models.
The final aim of this project is to build and analyse a unified Monte Carlo framework to solve ensemble optimal control problems governed by kinetic plasma models. The control is assumed to be located in the external force, in particular as an external magnetic field. Numerical experiments will be designed and executed that aim to successfully validate the optimisation framework.

Benchmark Quality Time-dependent Transport Solutions Using a Moving Mesh

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Abstract

Traveling discontinuities in the scalar flux can make accurate solutions to time dependent transport problems difficult to achieve. To obtain computationally inexpensive, accurate benchmark solutions, and eventually to solve radiation transfer problems with thermal feedback, we propose a novel Discontinuous Galerkin (DG) and discrete ordinates method. In this method, the spatial cell edges are time dependent, allowing them to track and resolve discontinuities in the scalar flux. Additionally, the method leverages the method of multiple flux decomposition and computes the collided portion of the flux using an analytic treatment of the uncollided particles as the source. Compared to a standard DG implementation, the solutions using a moving mesh and the analytic uncollided source give an error 875 times smaller on a plane pulse problem. Convergence result for a variety of test problems are shown in Fig.1.

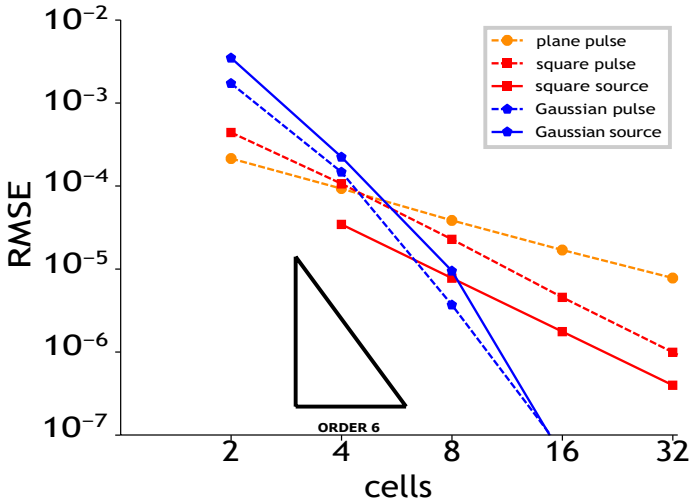

Figure 1: Logscale of root mean square error (RMSE) vs. number of spatial mesh subdivisions convergence results with a moving mesh, uncollided source method for five test problems

A general kinetic model of Boltzmann type for polyatomic gases

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Abstract

We propose a kinetic Boltzmann model for polyatomic gases, where the internal structure of a molecule is described by a single internal state parameter, belonging to a suitable space [1]. Proper options for such a space of internal states and for the measure defined on it allow to recover some models commonly used in kinetic theory for polyatomic particles: the description based on a set of discrete internal energy levels [2,3], and the one involving a continuous internal energy variable [4]. Moreover, within this general framework it is possible to build up new models desirable in physical applications, as a description able to separate the internal energy into two different components, the rotational and the vibrational ones, with the former approximated by means of a continuous variable, keeping the latter discrete. We prove the H-theorem for the proposed kinetic equation of Boltzmann type in this general framework, and we characterize the equilibrium Maxwellian distribution and the thermodynamic number of degrees of freedom. We also show how is possible to reduce some models fitting this general setting to a one-real-variable description with a suitable measure, similar to the classical continuous model with integration weight. Possible generalizations of our formulation to gas mixtures of polyatomic and monoatomic constituents, even in presence of bimolecular chemical reactions, are also discussed.

References

[1] T. Borsoni, M. Bisi, M. Groppi, A general framework for the kinetic modelling of polyatomic gases, *Commun. Math. Phys.* (2022), doi: 10.1007/s00220-022-04367-0.
[2] V. Giovangigli, *Multicomponent Flow Modeling,* Birkhäuser, Boston, 1999.
[3] M. Groppi, G. Spiga, Kinetic approach to chemical reactions and inelastic transitions in a rarefied gas*, J. Math. Chem.* **26** (1999), 197-219.
[4] L. Desvillettes, R. Monaco, F. Salvarani, A kinetic model allowing to obtain the energy law of polytropic gases in the presence of chemical reactions, *Eur. J. Mech. B Fluids* **24** (2005), 219-236.

Swarm formation

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Abstract

The formation of insect swarms has been studied experimentally and theoretically for decades [1-3]. The widely used Vicsek model consists of N particles moving with constant speed in a box with periodic boundary conditions and adapting their velocities at discrete times to a majority rule of their neighbors' plus noise [4]. Using a molecular chaos truncation, Ihle proposed a discrete-time Enskog-type kinetic theory of the Vicsek model and derived hydrodynamic equations [5]. We analyze swarm formation by deriving partial differential bifurcation equations for density and mean velocity from the Ihle kinetic theory [6]. The equations are hyperbolic on a short time scale and parabolic on a longer time scale. Their solutions include bands and wavetrain patterns agreeing with direct numerical simulations. The wavetrains have oscillation frequencies which we predict by using a linearization approximation [6]. The wave amplitudes increase with time for the hyperbolic system but are stabilized to finite values for the parabolic system [7]. We have also discovered a scale-free chaos phase transition for a harmonically confined three-dimensional Vicsek model [8] that explains observations on midge swarms [3].

[1] A. Okubo, Advances in Biophysics 22, 1-94 (1986).
[2] J. G. Puckett, N. T. Ouellette, J. Royal Society Interface 11, 20140710 (2014).
[3] A. Cavagna et al, Nature Physics 13, 914-918 (2017).
[4] H. Chaté, Annual Reviews Condensed Matter Physics 11, 189-212 (2020).
[5] T. Ihle, Physical Review E 83, 030901 (2011).
[6] L. L. Bonilla, C. Trenado, Physical Review E 98, 062603 (2018).
[7] C. Trenado, L. L. Bonilla, A. Marquina, arXiv:2203.14238.
[8] R. González-Albaladejo, A. Carpio, L. L. Bonilla, preprint 2022.

Analysis of the correlation functions for the neutron and precursor populations at criticality

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Abstract

Neutron populations in reactor cores at low densities might display highly non-Poissonian fluctuations close to criticality, due to fission-induced space and time correlations. Such fluctuations have been shown to be responsible for two peculiar phenomena: spontaneous spatial clustering, leading to a wild "patchiness" of the neutron population, and eventually a "critical catastrophe" where the typical size of a single fluctuation can attain the order of magnitude of the average concentration and make the entire population disappear. A milder behaviour is observed when some form of feedback (e.g., the Doppler effect) is taken into account: in particular, the critical catastrophe is then avoided and the fluctuations level off at an asymptotic amplitude. The investigation of these phenomena is of utmost importance for reactor start-up or shut-down operation, where the core is operated at low densities. The mathematical description of space and time-correlations can be carried out in the framework of neutron transport theory by resorting to the master equation yielding the joint probability $P(x_1, x_2, \ldots, x_n, t_1, t_2, \ldots, t_n)$ of observing a particle at position x_1 and time t_1, a particle at position x_2 and time t_2, etc. While the master equation is typically difficult to manipulate, having an extremely involved structure, useful information concerning the behaviour of the neutron fluctuations can be extracted from the associated low-ordermoments, i.e., the average concentration $c(x,t) = \langle n(x,t) \rangle$ and the two-point correlation function $h(x_1,x_2,t_1,t_2) = \langle n(x_1,t_1)\, n(x_2,t_2) \rangle$. In recent years we have provided a full characterisation of the two-point correlation function by building on pioneering work done by many authors, including Pál,Bell, Williams and Pázsit, and we have shown that this quantity is key to understanding both the patchiness and the critical catastrophe. In particular, we have derived a closed formula for the typical square distance between a pair of neutrons in the system, which yields the linear size of "neutron clusters" as a function of the physical parameters (cross sections, fission yield, etc.). A generalized equation taking into account an ideal feedback (corresponding to strict control with fixed population size) was also proposed. In this work, we will extend our previous results in several directions: first, we will include the presence of delayed neutrons (which for the sake of simplicity were not explicitly considered so far); second, we will relax the hypothesis of fixed population size and examine the broader cases where control is applied to neutrons alone or neutrons and precursors combined. Analytical or semi-analytical results for the concentration, the two-point correlation function and the pair distance will be derived and compared to Monte Carlo simulations, which will be used as a reference. We will show that both the presence of delayed neutrons and the use of population control mechanisms are extremely effective in reducing the amplitude of the correlation function and thus quenching neutron clustering.

1 CEA/ISAS/DM2S/SERMA/LTS

A Rational Extended Thermodynamics description of acceleration waves and oscillating gas bubbles

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Abstract

The study of acceleration waves [1] for a rarefied polyatomic gas is carried out in planar, cylindrical and spherical geometry referring to the rational extended thermodynamics theory with 14 moments [2]. The case of a rarefied monatomic gas is determined as a limit case, and the role of geometry and molecular degrees of freedom is investigated [3].
In addition, the behaviour of an acceleration wave travelling inside an oscillating gas bubble [4] is modelled by the 14-moment PDE system under adiabatic condition. We show that dissipation combined with hyperbolicity tends to inhibit shock formation, and that the dynamic pressure cannot be zero inside the oscillating bubble. This fact can produce observable effects even in the Navier-Stokes approximation, if the gas exhibits high bulk viscosity [3].

[1] Boillat G.,: *La propagation des ondes*. Paris, France Gauthier-Villars (1965). Ruggeri T.: *Stability and discontinuity waves for symmetric hyperbolic systems*. Nonlinear wave motion ed. A. Jeffrey, Longman, 148-161 (1989).
[2] Ruggeri T., Sugiyama M.: *Classical and Relativistic Rational Extended Thermodynamics of gases*. New York, Springer (2021).
[3] Brini F., Seccia L.: *Acceleration waves and oscillating gas bubbles modelled by rational extended thermodynamics*. Submitted (2022).
[4] Prosperetti A., Hao Y.: *Modelling of spherical gas bubble oscillations and sonoluminescence*. Phil. Trans. Royal Soc. A {\bf 357}, 203-223 (1999).

A bipolar hydrodynamical model for charge transport in graphene nanoribbons

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Abstract

Since its first isolation as a single layer of carbon atoms graphene has appeared as one of the most promising material for the new era of electronic devices [1,6]. It presents high electronic mobility at room temperature and high current density, nevertheless the absence of a band gap in its band structure does not make it a good solution for controlling the current flux. For solving the drawback the pristine graphene can be substituted by graphene nano-ribbons, narrow strips of graphene that exhibit a band gap depending on the width of the strip [2, 3, 7]. Here we propose a bipolar hydrodynamical model for the charge transport in graphene nano- ribbons that takes into account the gap in band structure and the electron scattering with the lattice structure and with the edge [4, 5, 6].

References

[1] A. H. Castro Neto, et al. The electronic properties of graphene, Rev. Mod. Phys, 109(81), 2009.

[2] L. Yang, C.-H. Park, et al. Quasiparticle Energies and Band Gaps in Graphene Nanoribbons, Rev. Mod. Phys, 186801 (99), 2007

[3] M. Bresciani, P. Palestri, D. Esseni, L. Selmi. Simple and efficient modeling of the E-k relationship and low-field mobility in Graphene Nano-Ribbons, Solid-State Electronics, 54, 1015–1021, 2010.

[4] V. K. Dugaev, M. I. Katsnelson. Edge scattering of electrons in graphene: Boltzmann equation approach to the transport in graphene nanoribbons and nanodisks, Physical Review B, 88, 235432, 2013.

[5] V.D. Camiola, G. Nastasi, Hydrodynamical Model fo Charge Transport in Graphene Nanoribbons, J. of Stat. Phys. (2021)

[6] V.D. Camiola, G. Mascali, V. Romano, Charge Transport in Low Dimensional Semiconductor Structures, Springer (2020)

[7] V.D. Camiola, V. Romano, Hydrodynamical model for charge transport in graphene, J. Stat. Phys. 157 (2021)

Kinetic models for angiogenesis: analysis and simulation

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Abstract

Angiogenesis (growth of blood vessels) is fundamental for tissue development and repair. Numerous inflammatory, immune and malignant diseases are fostered by angiogenic disorders. Hypoxy induced angiogenesis processes including the effect of stochastic motion and branching of blood vessels can be described by an integrodifferential kinetic equation of Fokker–Planck type with source terms that are nonlocal in time, coupled with a diffusion equation for the angiogenic factor [1]. Such models admit soliton-like asymptotic solutions representing the advance of the blood vessels towards the hypoxic regions, such as tumors [2]. We establish the well posedness of the model in the whole space by first constructing the Green functions (fundamental solutions) for the underlying transport problems with variable sources and establishing estimates for their key decay properties [3]. We then implement an iterative linearized scheme whose solutions converge to solutions of the original model, as it follows from comparison principles, sharp estimates of the velocity integrals and compactness results for this type of kinetic and parabolic operators. In bounded domains, the kinetic equations are supplemented with nonlocal boundary conditions and coupled to a diffusion problem with Neumann boundary conditions through the force field created by the tumor induced angiogenic factor and the flux of vessel tips [4]. Lacking explicit expressions for the Green functions, well posedness results exploit balance equations, estimates of velocity decay and compactness results for kinetic operators, combined with gradient estimates of heat kernels for Neumann problems. Our well posedness studies underline the importance of preserving positivity in the schemes employed to approximate numerically solutions. We are able to construct numerical solutions devising order one positivity preserving schemes and show that soliton-like asymptotic solutions are correctly captured [5]. We also find good agreement with the original stochastic model from which the deterministic kinetic equations are derived working with ensemble averages. Higher order positiviy preserving schemes can be devised comibining WENO (weighted essentially non oscillatory) and SSP (strong stability preserving) discretizations [6].

References

[1] F. Terragni, M. Carretero, V. Capasso, L. L. Bonilla, Stochastic model of tumor- induced angiogenesis: ensemble averages and deterministic equations, Phys. Rev. 93, 022413, 2016

[2] L. L. Bonilla, M. Carretero, F. Terragni, Solitonlike attractor for blood vessel tip density in angiogenesis, Phys. Rev. 94, 062415, 2016

[3] A. Carpio, G. Duro, Well posedness of an integrodifferential kinetic model of Fokker-Planck type for angiogenesis, Nonlinear Analysis-Real World Applications 30, 184-212, 2016

[4] A. Carpio, G. Duro, M. Negreanu, Constructing solutions for a kinetic model of angiogenesis in annular domains, Applied Mathematical Modelling 45, 303-322, 2017

[5] L.L. Bonilla, A. Carpio, M. Carretero, G. Duro, M. Negreanu, F. Terragni, A convergent numerical scheme for integrodifferential kinetic models of angiogenesis, Journal of Computational Physics 375, 1270-1294, 2018

[6] A. Carpio, E. Cebrián, Positivity preserving high order schemes for kinetic models of angiogenesis, International Journal on Nonlinear Sciences and Numerical Simulation, 2022, to appear, https://doi.org/10.1515/ijnsns-2021-0112

First-Collision Source Treatment for Ray Effect Mitigation in Discrete-Ordinate Radiation Transport Solutions

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Abstract

Deterministic transport codes play a fundamental role in the modeling and simulation of neutron transport. One of the most common deterministic methods is the method of discrete ordinates, also known as the S_n method. While offering significant advantages over other deterministic methods or stochastic methods like Monte Carlo, the method of discrete ordinates suffers from non-physical artifacts in its local solution due to its discretization of angle. These artifacts, referred to as ray effects because of their ray-like appearance, tend to be worse in problems with small sources in areas with little scattering. Significant effort has gone into developing methods to mitigate ray effects, such as the first-collision source treatment, which separates the angular flux into the uncollided and collided fluxes and solving them using non-traditional techniques such as ray tracing. One such code capable of doing this is Lawrence Livermore National Laboratory's deterministic transport code ARDRA. Current ray tracing methods typically trace to a set of points inside a zone to compute an overall flux. However, this approach has significant drawbacks, such as a low order of convergence and not being conservative. Therefore, a new method has been developed that traces instead to a set of points on each of a zone's surfaces and computing the currents, before using these to obtain the flux. A comparison between these two ray tracing methods showed significant advantages to the new surface method, including inherent conservation, a higher convergence rate, and an increase in calculable information like leakage.

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Multi-cue kinetic model for cell migration on a fiber network

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Abstract

In several physiological and pathological situations, cells perform directed motion in response to external stimuli by sensing the environment with their membrane protrusions. Precisely, several biochemical and biophysical cues give rise to direct migration towards specific targets. This defines a multi-cue environment in which cells have to sort and combine different, and potentially competitive, stimuli. Following [1,2], we develop a non-local kinetic model for cell migration in which cell polarization is influenced simultaneously by the fiber network and a chemotactic agent. Analyzing two possible sensing strategies, we define the corresponding transport models and we recover the appropriate macroscopic limit in different regimes, depending on the relation between the cell size and the variation of the external fields [3]. We numerically integrate the kinetic transport equations in a two-dimensional setting and we qualitatively investigate various scenarios. In particular, we show how our model is able to reproduce experimental results concerning the influence of topographical and chemical cues in directing cell motility. Moreover, we extend the setting to include situations in which cell migration is physically limited by the presence of dense fibrous regions affecting cell speed and we analyze the corresponding model combining contact guidance and steric hindrance from a microscopic and a kinetic viewpoint [4].

References:

1. Loy, N., & Preziosi, L. (2020). Kinetic models with non-local sensing determining cell polarization and speed according to independent cues. *J. Math. Biol.*, **80(1)**: 373-421.
2. Loy, N., & Preziosi, L. (2020). Modelling physical limits of migration by a kinetic model with non-local sensing. *J. Math. Biol.*, **80(6)**: 1759-1801.
3. Conte, M., & Loy, N. (2022). Multi-Cue Kinetic Model with Non-Local Sensing for Cell Migration on a Fiber Network with Chemotaxis. *Bull. Math. Biol.*, **84(3)**: 1-46.
4. Conte, M., Loy, N., & Preziosi, L. (2022). A non-local kinetic model for cell migration on the extracellular matrix by contact guidance and steric hindrance. In preparation

Implementation of the Random Ray Method in the Monte Carlo codes SCONE and OpenMC

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Abstract

The Random Ray Method (TRRM) is a stochastic algorithm which has been successfully applied to multi-group neutron transport problems. It is based on the standard Method of Characteristics (MoC) but uses a stochastic quadrature that varies each iteration, as opposed to the usual deterministic quadrature. Several publications have demonstrated the significant promise of TRRM against 3D MoC with regards to geometric flexibility, reduced memory requirements, and superior numerical performance. Arguably, one of the most involved aspects of TRRM is the geometry engine, namely the ability to efficiently calculate track lengths in the direction of flight across general reactor geometries. However, this is necessarily done natively in most Monte Carlo particle transport codes. As such, this paper demonstrates the straightforward implementation of TRRM in two open-source Monte Carlo codes, SCONE and OpenMC, and compares their performance against multi-group Monte Carlo on the C5G7 multi-group benchmark problem. Preliminary results show a substantial speed-up which is expected to improve further in problems with larger numbers of energy groups.

On the accuracy of the Ronen Method in plane geometry

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Abstract

The Ronen method (RM) was introduced in diffusion theory with the goal of finding more accurate solutions, with transport theory as a reference. In this method, a transport equation of integral type provides an expression for the net current that is used in an iterative and nonlinear scheme to force the solution from diffusion to fulfil the same integral equations. The method was also formulated by using the formalism of collision probability method, still without any operator inversion other than the one used by diffusion. The RM was tested on a complete suite of one-dimensional multigroup benchmark problems, in multiple geometries. Despite the upgrade of the iterative scheme with the damped Anderson acceleration (DAAREM), needed because of general slow convergence, there were still differences in the flux with reference solutions from transport. The differences, though small, appear at material interfaces and close to boundary with vacuum, that is where transport effects are more pronounced. In this work, we present the preliminary results obtained from investigations carried out to explain these differences. An approach based on the use of reference solution by transport is introduced in the homogeneous and heterogeneous finite slab to cast the solution with the diffusion approximation on transport. Specifically, an optimal diffusion coefficient is defined, and a redefinition of the extrapolated distance is also introduced by using Fick's law and the solution from transport (collision probability method). For the homogeneous case, a diffusion coefficient formulation, based on the derivation of the diffusive contribution of the exact transport solution obtained by Case's method is also introduced. Simple diffusion and diffusion corrected by RM are tested using these new quantities as input parameters. Eventually, closer results to transport are found, meaning that corrected diffusion can reproduce transport on the condition of using optimal coefficients.

Keywords: Ronen method, neutron transport approximation, diffusion coefficient

Step Correlations in Non-Classical Transport using 1D Point Processes

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Abstract

We propose a new model for monoenergetic linear transport in stochastic media where successive free-path lengths between collisions can be correlated. In our model, the collision times of a particle are determined by a 1D point process chosen such that perfectly forward scattering along a transect exactly matches ensemble-averaged statistics. Application of this point process to problems with general scattering is approximate but more efficient than a double-Monte-Carlo benchmark simulation. This approach increases in accuracy as the phase function peaks forward (common for light transport problems) and becomes exact for perfectly forward scattering. We derive an integral formulation of our transport model that includes renewal transport processes (classical radiative transfer, non-exponential random flights, tightly-coupled continuous time random walks and the generalized linear Boltzmann equation), Markov-renewal transport processes (the chord-length-sampling method for Markov binary mixtures), and Mixed-Poisson transport processes (the independent column approximation) as special cases. Previous renewal formulations of non-classical radiative transfer only ensure that the first collision time is exact and assume subsequent collision times are independently and identically distributed. By supporting non-renewal collision times, our model can account for the step correlations that arise in most variability models, including cross-section fluctuations driven by Gaussian processes, transformed Gaussian processes, and most discrete mixture models. We compare multiple scattering predictions of our model to benchmark solutions for Gaussian and transformed Gaussian fluctuations in a Flatland domain and demonstrate improved accuracy relative to renewal approximations. The narrow conditions under which a continuum description of fluctuating cross sections (Cox processes) are also renewal processes is discussed.

On a regime-switching stochastic epidemic model for COVID-19

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Abstract

The COVID-19 pandemic has unpredictable comportments and is persisting in some countries. Its spread could depend on exogenous factors. But most of the recent stochastic epidemic models do not treat outsider events. In this work, we aim at investigating a stochastic epidemic SIR model for covid-19 where the impact of an external event is embedded in the model. The paper considers a regime-switching continuous stochastic epidemic model where two independent sources of randomness are governing the model: a Brownian motion and a continuous-time Markov chain process modelling the exogenous event. After introducing the model, the existence and uniqueness of positive solutions are proved. Then we deal with the extinction, as well as persistence analysis, where we get the conditions on extinction and persistence. Numerical simulations are conducted and some illustrations are provided.

A Novel Angular Discretization method for the Neutron Transport Equation: the MPN method

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Abstract

The accuracy of the angular discretization in the deterministic solution of the transport equation is particularly relevant for radiation shielding calculations. It is demonstrated how the Discrete Ordinate (S_N) method, commonly used in reactor core simulations, turns out to be inefficient in the presence of geometrically large and low-scattering regions, giving rise to the so-called ray-effect. This is a symptom of insufficient angular discretization, and appears to be extremely persistent with respect to the refinement of the angular quadrature formula.
The Multi-P_N method (MP_N) lends itself well as a possible alternative to Discrete Ordinates. It stands halfway between S_N and the Spherical Harmonics methods, as it preserves the block-diagonal structure of the discretized displacement plus removal operator, yet introducing an angular expansion of the interface fluxes. The method is derived from the integral formulation of the transport equation, discretized in space by the short characteristics method. By defining an angular decomposition of the unit sphere into solid angles, and then a local polynomial angular basis within each solid angle, it is possible to project the short-characteristic equations on this angular base to obtain a new formulation of the transport equation, coupling more than one angular degree of freedom within the same solid angle. This coupling, being local, enables to solve the equation by means of a standard sweep algorithm. Therefore, its implementation requires a reduced number of variation with respect to the common S_N solver.
The enriched angular coupling allows for a mitigation of the ray effect. Furthermore, the formulation thus obtained does not imply any angular quadrature rule, like in S_N. Instead, the angular moments of the flux are directly computed by projecting the integral formulation onto the space of spherical harmonics.
Tests conducted with MP_N on particle propagation problems affected by ray-effect show better performances than those obtained with S_N. The MP_N numerical solutions are less affected by the ray-effect and the measured convergence rate with respect the angular degrees of freedom is significantly larger than the one measured with S_N.

Efficiency calibration of a stable NaI(Tl) detector for ^{41}Ar for air exhaust systems

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Abstract

Positron Emission Tomography (PET) is a functional imaging technique and has become a significant tool for diagnostic purposes in the field of oncology in recent years. While the production of radioisotopes used for PET imaging can lead to the production of radioactive gases which need to be monitored before releasing to the environment. ^{41}Ar is an essential gaseous radionuclide that must be monitored in gaseous effluents from nuclear facilities. Therefore, a precise evaluation of ^{41}Ar activity is highly desired. Multichannel analyzers (MCA) are widely used to investigate different sources and samples with a long available time of analysis. One of the most widely used instruments consists of a NaI(Tl) scintillation detector coupled with a Multi-Channel Beacon (MCB). However, a critical issue is that the environmental parameters can affect its performance and the relevant analysis software does not consider the possible channel drifting effects. On the other hand, efficiency calibration of these kind of monitoring systems are highly depends on the source-detector geometry and it may make the calibration complicated with large amount of uncertainty. So, Monte Carlo simulation can be a suitable approach for evaluating the detector efficiency. The main aim of this study is to evaluate the full peak efficiency of a 2" × 2" NaI(Tl) scintillation detector for a ^{41}Ar source with 1293.5 keV energy in two different source-detector geometries as duct and Marinelli beaker using the FLUKA code. Moreover, a new experimental technique was considered to produce ^{41}Ar standard source with specific activity in a controlled geometry like Marinelli beaker through neutron irradiation of natural argon inside a cyclotron bunker. ^{41}Ar gamma spectrum was acquired using a 2" × 2" NaI(Tl) coupled with a stable MCA. The MCA stability was investigated in different temperatures and relative humidity conditions. The simulation data were compared with the experimental results for Marinelli beaker geometry, and the ratio was evaluated as 0.99±0.07. The ratio was considered as a scaling factor for the final efficiency calibration of duct geometry.

Full Recovering of an X-ray Spectrum from Detector Influence

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Abstract

It is well known that a measured energy dispersive X-ray spectrum differs from the original spectrum arriving to the detector. This is due to changes introduced by the detection device and by the pulse electronics during the measurement. The detection device contributes with a deformation attributed to the detector response function (DRF) which is well described in terms of physical processes of radiation diffusion inside the detector. The pulse electronics contributes in two different ways: (a) with a convoluted broadening due to an asymmetrical distribution at each recorded energy (resolution effect) which produces an uneven smoothing of the spectrum, and (b) with the pulse pile-up which introduces a distortion which changes the total counts and the shape of the spectrum. Once characterized the DRF comprising the resolution broadening effects, it is possible to recur to an unfolding algorithm to recover the original spectrum.

In this paper it is introduced a detailed description of the four steps which are necessary to recover the source spectrum from a measurement by using a set of computer codes developed in Bologna. In first place, it is applied a PPU correction algorithm on the measured spectrum which renders a corrected measure having the proper number of counts in the proper energies. Then it is computed the combined effect of the DRF and the asymmetrical resolution for each energy of the source spectrum. By discretizing these single energy distributions, it is possible to obtain the response matrix feeding the next step. The last step consists in the application of a robust unfolding procedure like UMESTRAT, the maximum entropy technique which takes advantage of the known a priori information and preserves the positive-defined character of the X-ray spectrum.

The results obtained are very good and are illustrated with some paradigmatic examples involving popular SSDs like Si, Ge and CdTe.

Numerical Caseology by Lagrange Interpolation for The 1d Neutron Transport Equation In A Slab

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Abstract

We are concerned with a new, highly precise, numerical solution to the 1D neutron transport equation based on Case's analytical singular eigenfunction expansion (SEE). While a considerable number numerical solutions currently exist, understandably, because of its complexity, even in 1D, there are only a few truly analytical solutions to the neutron transport equation. In 1960, Case introduced a consistent theory of the SEE for a variety of idealized transport problems and forever changed the landscape of analytical transport theory. What is presented is yet another, called the Lagrange order N method (LNM), featuring the simplicity and precision of the FN method, but for a more convenient and natural Lagrangian polynomial basis.

The value of Caseology, is mainly theoretical to enable the solution of the transport equation to as close to a closed form exact solution as possible. For monoenergetic neutron transport with isotropic scattering, exclusively considered here, there are only a handful of problems that lend themselves to closed forms, *i.e.*, primarily transport in an infinite medium and a half-space. A second advantage of Caseology, is the foundation it provides to develop highly precise numerical solutions, such as the FN method. To the author's knowledge, the numerical solution, to be presented, is different from those found in the literature. When expressed as the full-range SEE, the solution for the slab is no longer in a closed form unlike for infinite media. Its evaluation involves iteration through auxiliary X- and Y- functions as in invariant imbedding or a Fredholm integral equation, which solve non-linear coupled integral equations. The same is true for the half-space to determine the Case X-function (or equivalently Chandrasekhar's H-function), but unlike the slab, these functions have closed form integral representations. Our goal is to avoid evaluation of the auxiliary non-linear integral equations for the slab and remain true to the original form of the full-range SEE. While SEE is not the only way to find analytical solutions, in comparison to Weiner-Hopf, invariant imbedding, Laplace and Fourier transforms, this author believes it to be the most mathematically pleasing.

We begin by representing Case's solution in terms of the discrete and singular eigenfunctions for an isotropically scattering slab. The known incoming flux entering the slab surfaces provide two coupled singular equations for the expansion coefficients. By adding and subtracting, the equations uncouple to give a combination of just the continuum coefficients in terms of the discrete. In addition, superposition eliminates the dependence on the discrete coefficient enabling the continuum coefficients to be determined independently from the discrete. The discrete coefficients come from orthogonality requiring integration over the continuum coefficients already found by combining Lagrange interpolation with GQ.

Table 1 gives a demonstration for the variation c for a 1mfp slab. Here, one observes the degradation of the LNM because of its inability to fully capture ν_0. as c nears 0.1. Only 6-place precision is achievable for $N =$ 2500, which is extreme for 1D transport calculations. For the remainder of the table (of quadrature order 600) only four digits are missed by one unit in the ninth place.

Table 1. Exiting Flux variation with c for $\Delta = 1$

$\mu\backslash c$	0.1	0.3	0.5	0.7	0.9	0.99
-1.0000E+00	1.504005***72***E-02	5.124571442E-02	9.911918554E-02	1.660168888E-01	2.674103351E-01	3.329218166E-01
-8.0000E-01	1.751883***83***E-02	5.955471562E-02	1.148847489E-01	1.918241465E-01	3.078331616E-01	3.825130896E-01
-6.0000E-01	2.092893***10***E-02	7.088964428E-02	1.361760310E-01	2.262501843E-01	3.609294436E-01	4.471117240E-01
-4.0000E-01	2.586115***47***E-02	8.702979248E-02	1.659221624E-01	2.732166375E-01	4.311708733E-01	5.311207558E-01
-2.0000E-01	3.353614***47***E-02	1.112934854E-01	2.087387645E-01	3.370749686E-01	5.194020596E-01	6.317828084E-01
0.0000E+00	5.128273***71***E-02	1.628491538E-01	2.904737980E-01	4.423922290E-01	6.353636392E-01	7.447453683E-01
0.0000E+00	8.028514***627***E-03	2.866250776E-02	5.854426***75***0E-02	1.045295474E-01	1.815479981E-01	2.348508***61***3E-01
2.0000E-01	1.813781***93***E-02	4.764831***99***E-02	9.062607009E-02	1.568687***20***8E-01	2.675980096E-01	3.440071157E-01
4.0000E-01	9.550016***20***E-02	1.294549833E-01	1.774911944E-01	2.494526695E-01	3.664802865E-01	4.458002699E-01
6.0000E-01	2.021168***62***E-01	2.352555191E-01	2.814495411E-01	3.496391717E-01	4.589432518E-01	5.323251387E-01
8.0000E-01	2.988610467E-01	3.295973198E-01	3.720980262E-01	4.343264153E-01	5.332715234E-01	5.993412930E-01
1.0000E+00	3.792294807E-01	4.073575782E-01	4.460583899E-01	5.024362348E-01	5.916250896E-01	6.509775491E-01

Response Matrix Discrete Ordinates Solution of the 1D Fokker-Planck Equation

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Abstract

Appropriate characterization of particle scattering is crucial in any reliable transport application. For neutrons, there is the scattering phase function, which generally is expressible as a Legendre polynomial expansion and is mildly forward peaked. We apply the response matrix method of solution RM/DOM[1] previously applied for neutron and photons with mild to extreme forward peaked scattering. In extreme forward scattering however, such as required for detection of tumors by light scattering or for screen-Rutherford scattering of electrons in cancer treatment, Fokker-Planck scattering could be effective. Thus, our focus of this work is on a new and effective application of response matrix theory of the Fokker Planck Equation (FPE).

We begin by choosing the discrete ordinates and their ordering, determined by the SN balance equation incorporating the discrete version of the directional FP operator [2]. The formal exponential solution, leads to the evaluation of the matrix exponential through diagonalization, which we show to be equivalent to a spectral eigenfunction expansion the numerical evaluation of which is unstable. To stabilize, we introduce a stabilizing factor. A straightforward numerical evaluation of the vector equation, identical to the solution found in Ref[2], follows achieving nearly five-place precision for reflected and transmitted intensities, which defines the tumor response.

The precision and stability of the numerical solution provides an opportunity to investigate feasibility of detecting tumors through optical means. Consider an isotropic beam of intense light impinging on a tissue sample in which a tumor exists as shown in the following figure:

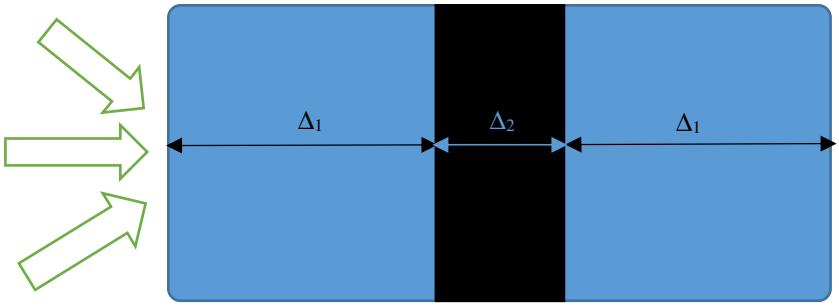

Fig. 1 Tissue sample with tumor (black).

The sample geometry assumes a slab medium with three contiguous regions of healthy and tumor infected tissue. In our study, we assume the tumor is a highly forward peaked scattering medium; while, the surrounding healthy tissue, otherwise identical, is much less forward peaked. One anticipates that because of the scattering contrast, the tumor will cause a perturbation of reflected and transmitted light. We obtain the response for the three-cell combination by determining the response for the first two cells separately and combining that response with the third cell.

We now simulate tumor detection based on tumor width. Figure 2 shows results for the variation of tumor widths Δ_2 to identify sensitivity to tumor forward peaked scattering. The sample total thickness is $1cm$ and the size of the tumor, located at the sample center, varies from 10 to 100% of the sample.

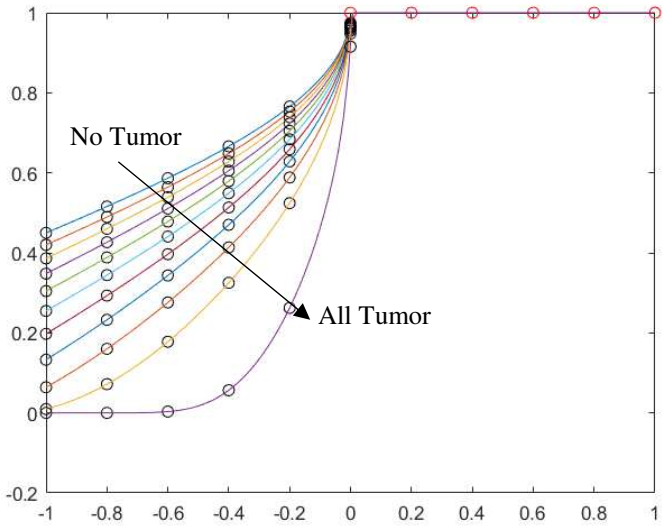

Fig. 2. Tumor reflected intensity response.

The tumor response to its thickness variation is quite apparent, indicating size detection via FP scattering of intense light may indeed be feasible.

On the statistical model of the atom

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Abstract

The Thomas-Fermi statistical model for the ground state of an atom was used for the determination of the non-uniform electron density $n(r)$ and of the self-consistent electric field $V(r)$ within the atom. This model assumes that the functions $n(r)$ and $V(r)$ vary slowly enough within an electron De Broglie wavelength, so that the "quasi-classical" description can be used.

The original approach, followed by many, about this subject was first to apply statistics to the fully degenerate non-uniform electronic cloud of a heavy atom. Then a Poisson equation for the self-consistent field (or mean field) of the cloud is obtained but, due to its difficulties, it was previously solved (see also Feynman, Metropolis, Teller; March, and other references) only numerically.

The Thomas-Fermi model has since then proved to be very useful in deriving properties such as the binding energy of heavy atoms. Besides, after suitable modifications, it has been applied to molecules, solids and nuclei. (see e.g. C. Bernardini, C. Guaraldo Fisica del Nucleo, Editori Riuniti, Roma, Italy 1994)

In this work we propose a different approach, starting from the Fermi-Dirac distribution function. Upon a suitable approximation of the inhomogeneous electron density, we give an exact solution of the Poisson equation. This yields a better insight about the physics of the problem and allows to obtain, not only $n(r)$ and $V(r)$, but also the ionization energy and the discrete energy levels of the completely degenerate cloud of electrons in the extra-nuclear space of the atom. In addition, we get the chemical potentials and the radii of the heavy atoms.

A mixed BGK-Boltzmann model for inert gas mixtures

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Abstract

Relaxation-time approximations of BGK-type constitute the most used simplified kinetic models of the Boltzmann equations of Rarefied Gas Dynamics, since they retain the most significant mathematical and physical features of the Boltzmann description. The extension of the BGK model to a gas mixture is not unique, since Maxwellian attractors in the BGK relaxation term depend on several free parameters in this case. The BGK models available in the literature may be divided into two classes, the former assuming the kinetic equation for each species governed by a unique relaxation operator [1,2], and the latter showing a sum of binary relaxation operators, preserving thus the structure of the original Boltzmann system [3]. BGK models [1,2,3] for inert mixtures have been recently compared also numerically, using suitable asymptotic preserving, conservative semi-Lagrangian schemes [4].

In order to preserve as much as possible the accuracy of the Boltzmann description, but with a kinetic system manageable from the computational point of view, we propose a mixed Boltzmann-BGK model for gas mixtures. In this setting, collisions occurring within the same species (intra-species) are modelled by Boltzmann operators, while interactions between different components (inter-species) are described by the BGK operators given in [3], that represent the relaxation model for mixtures with the closest structure to the Boltzmann one. We prove consistency of the model: conservation properties, positivity of all temperatures, H-theorem, and convergence to a global Maxwellian equilibrium with all species sharing a common mean velocity and a common temperature. We also derive hydrodynamic equations in different collisional regimes (with all collisions dominant, or with only collisions within the same species playing the dominant role). Some results relevant to this mixed Boltzmann-BGK model for a mixture of only two species [5] are presented.

REFERENCES

[1] P. Andries, K. Aoki, B. Perthame, Journal of Statistical Physics, 106, pp. 993-1018 (2002).

[2] M. Bisi, M. Groppi, G. Spiga, Physical Review E, 81, 036327 (2010).

[3] A. V. Bobylev, M. Bisi, M. Groppi, G. Spiga, I. F. Potapenko, Kinetic and Related Models, 11, pp. 1377-1393 (2018).

[4] S. Y. Cho, S. Boscarino, M. Groppi, G. Russo, Kinetic and Related Models, 14, pp. 895-928 (2021).

[5] M. Bisi, W. Boscheri, G. Dimarco, M. Groppi, G. Martalò, A new mixed Boltzmann-BGK model for mixtures solved with an IMEX finite volume scheme on unstructured meshes (submitted).

Discrete implicit Monte-Carlo (DIMC) scheme for simulating radiative transfer problems

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Abstract

One of the well-known methods for solving radiative transfer problems is using statistical Monte-Carlo techniques, specifically the implicit Monte-Carlo (IMC) of Fleck and Cummings [1]. This algorithm enables the use of large time steps, replacing the process of absorption and black-body emission in opaque materials, with an *effective* isotropic scattering term. This algorithm, with some modifications is being used during the last five decades.

However, the basic algorithm suffers from a well-known numerical error, that causes teleportation in optically-thick materials. When photons enter an opaque cell (specifically, a "cold" cell), they are absorbed in the outer part of the numerical cell and heat the material. Afterwards, in the next time step, the heated cell emits photons uniformly from the cell, which causes the photons to propagate faster than they should, i.e., *teleport*. Of course, this numerical issue converges with spatial resolution and time-step, however, in practice, the convergence is slow.

One promising method to eliminate the teleportation error, named Semi-Analog MC (SMC), was introduced by Ahrens & Larsen [2]. In this method, there are two types of particles, radiation photons and material particles. Instead of creating radiation photons from the thermal energy of the cell, the material particles have a chance to transform into radiation photons, and when radiation photons are absorbed they are transformed into material particles. Unfortunately, the explicit nature of the scheme forced very small time steps and made the method unappealing. A breakthrough was introduced recently by the milestone work of Poëtte and Valentin [3], where an implicit version of SMC (ISMC) was derived. We have explored the ISMC algorithm in many 1D and 2D problems (XY and RZ), both in gray and multi-group benchmarks [4]. The ISMC algorithm exhibited no teleportation errors compared to the IMC algorithm, and thus, converged much faster in spatial resolution and time-step.

Nevertheless, the ISMC results yield nosier solutions, due to the discrete nature of the absorption-emission process. Although it achieves a fast convergence in spatial resolution and time-step, ISMC requires many more particles for yielding IMC-like smooth results. In addition, in cases where there is a large ratio between the heat capacities of the radiation and the material, ISMC suffers from low statistic errors, and may require a prohibitively large number of particles.

In this work, we derive a new Monte-Carlo algorithm, Discrete implicit Monte-Carlo (DIMC) that uses the idea of the two-kind discrete particles and thus, does not suffer from teleportation errors effects on the one hand, and yields smooth results on the other hand [5]. DIMC implements the IMC discretization and creates new radiation photons each time step, unlike ISMC. Using the continuous absorption technique, DIMC yields smooth results as classic IMC. One of the main parts of the algorithm is the avoidance of population explosion of particles, using particle merging. We test the new algorithm in several one and two-dimensional cylindrical problems, and show that it yields smooth, teleportation-free results.

References:

[1] J.A. Fleck and J.D. Cummings, *JCP*, **8**, 313 (1971).
[2] C. Ahrens and E. Larsen, “A semi-analog Monte Carlo method for grey radiative transfer problems”, *M&C* (2001).
[3] G. Poëtte and X. Valentin, *JCP*, **412**, 109405 (2020).
[4] E. Steinberg and S.I. Heizler, *JCP* (2021).
[5] E. Steinberg and S.I. Heizler, *ApJS,* (2021).

Neutron Count Probability Approximations Using Moments, Meixner Polynomial Expansion and N-Forked Approximation

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Abstract

Because fission neutrons are time correlated, the statistical processing of neutron counting measurements makes it possible to detect and characterize nuclear materials. The number of detected neutrons recorded during a time interval is the basis of most of these techniques.

Considering simulations, the equations of counting probabilities and binomial moments are derived using the Kolmogorov backward methodology developed by Pál and Bell. With the exception of the zeroth order, the probabilities and moments equations are similar and can be solved successively using recurrence relations (Leibnitz formula for the derivatives of compound functions and Panjer's recurrence applied to generalized Poisson distributions).

Usually, the first moments are easier to calculate than the full probability distribution, especially when the count rate is large. Moreover, the probability of zero detection is solution of a non-linear equation while the moment or order zero is just equal to unity. For these reasons, we are interested in the approximation of the count distribution from its first moments only. Two methods are considered; the expansion of the distribution on a basis of Meixner discrete orthogonal polynomials and the N-forked approximation.

Meixner polynomial expansion is justified by the fact that the count distribution is known to be close to the Polya distribution which is the measure associated to Meitner polynomials. We present the computation of Meixner polynomials as well as the coefficient of the expansion which depend on the binomial moments of the target distribution. The Kth order expansion has the same K first moments as the target distribution. The first approximation (K=2) is the Polya's law having the same two first moments as the target distribution.

In the point model, the time dependent, two forked (quadratic) approximation of the count distribution with a Poisson source is the PMZBB approximation (Pál, Mogil'ner, Zolotukhin, Bell, Babala). The Poisson radical distribution introduced by N. Pacilio is a stationary PMZBB distribution parameterized by the first two moments. We have studied the extension of this method using up to four statistical moments (three and four forked correlations).

Finally, we present numerical test cases with different levels of multiplication, source intensity and detection efficiency. The results indicate that the reference distribution is well approximated as long as the level of detection efficiency and multiplication is not too high. Moreover, the N-forked approximation is generally more accurate than Meixner polynomial expansion for a same number of statistical moments used.

Entropy-stable Galerkin methods for the Boltzmann equation

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Abstract

In this talk, we develop an entropy-stable finite-element-moment method for the Boltzmann equation with full collision operator. To that end, we employ a discontinuous-Galerkin method in space and time, and a moment method in velocity. We base our method on a converging sequence of approximations to the collision operator. We associate with each member of this sequence a normalisation map for the distribution function and an entropy. We show that each approximate collision operator inherits salient properties from Boltzmann's operator, such as the preservation of the collision operator, the H-theorem and that the linearisations near equilibrium agree. We prove that our method is entropy-stable for each member of the sequence of approximations to the collision operator. Finally, we apply our method to the Boltzmann equation with full collision operator and demonstrate the corresponding approximation properties, using benchmark test cases, in comparison to Direct Simulation Monte Carlo.

About the construction of finite element bases on 3D hexagonal geometries for neutron transport simulation.

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Abstract

In order to solve partial differential equations on polygons, one way is to use the finite element method. However, developing high order finite element bases on 3D polygonal meshes is not trivial. In the particular case of 3D prismatic meshes (cylinders with any 2D base), such bases can be obtained by combining 2D radial basis functions and 1D basis functions (along the extrusion axis). The 3D basis is usually generated by the Cartesian product between these two functions sets to span a given three-dimensional polynomial space of order k (P_k). An important remark is that the resulting 3D basis spans a larger space: in fact, it is the space of polynomials with monomials of partial degree less than or equal to k (Q_k) that is spanned. In the frame of neutron transport simulation, it has been observed that the extra degrees of freedom offered by Q_k are often superfluous and have no significance in the subsequent interpolation for estimating the projected physical quantities.

Consequently, in an effort where the usual trade-off between computational accuracy and burden is targeted, it may be interesting to reduce the number of degrees of freedom. It is achieved by spanning as closely as possible P_k through other means than the basic Cartesian product of two spaces. In the particular application of reactor physics, this approach is acceptable as the radial and axial coupling of quantities is relatively low.
First, it is shown that P_k is included in the approximation space equals to the union (over $0 \leq n \leq k$) of 2D bases of order n times (Cartesian product) 1D bases of order $k - n$. Then, a hierarchical basis is

chosen for the 1D axis so that can be decomposed as a direct sum of $k + 1$ sets with the n-th set containing one single polynomial function of order n. Accordingly, to further reduce the degrees of freedom of the 3D approximation space, this research work proposes to construct as the direct sum (over $0 \leq n \leq k$) of 2D bases of order n times (Cartesian product) the 1D axial function of order $k - n$.

In our case, we have applied these bases to solve the neutron transport equation discretized by a discontinuous Galerkin method on 3D-extruded hexagonal meshes, which are required to model some reactor cores with hexagonal geometry. First, we have developed high-order finite element basis for the hexagon. Amongst various possibilities, we choose to use nodal rational finite element bases such as Wachspress bases. For the 1D bases, the Legendre polynomials have been chosen. Once the 3D bases generated by combining these 2D-1D bases, we then applied the method of manufactured solutions with the function $f(x, y) = sin(\alpha x)sin(\beta y)sin(\gamma z)$ with $\forall(\alpha, \beta, \gamma) \in \mathbb{R}^3$. The aim is to ensure that the approximated solution verifies the *a priori* estimate from the discontinuous Galerkin discretization, and thus the numerical orders of convergence in asymptotic regime are closed to the theoretical ones. Numerical results have been performed and give the expected results.

A new V&V philosophy for fusion nuclear data libraries

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Abstract

Up to 500 words, Times New Roman 12, single spacing

Cross sections evaluation is a long-thought process performed by a restricted number of field experts. This happens not only because this is a very difficult process which requires a lot of previous experience, but also because once a new release of nuclear data libraries is proposed, it needs to undergo costly extensive processes of Verification & Validation which, for the most part, are done manually. In the field of nuclear data for fusion applications, this process is even slower due to the fact that the majority of the effort is provided "in-kind". In this work, a new philosophy to approach nuclear data libraries evaluation and V&V is discussed, one that would leverage three modern pillars of computer science: open-source, continuous integration and machine learning. The first step to move towards this new philosophy has already been taken with the development of JADE [1][2]. JADE is the result of a collective effort between University of Bologna, NIER Ingegneria and Fusion For Energy and is a python-based software able to automatically generate, run and post-process an expandible number of computational and experimental transport benchmarks for the Verification and Validation (V&V) of nuclear data libraries, with a focus on fusion applications. First, the modifications that need to be applied to the code for it to be fully open-source will be discussed. Then, the strategy to move from a discrete release of new nuclear data (every few years) to one that implements continuous integration will be illustrated. This involves the use of JADE constantly running in cloud its benchmarks suite in order to verify new data that can be pushed to the library at any time. Finally, it will be discussed how the recent rise in the available computing power and near-future switch of Monte Carlo codes to GPU architecture could lead to new strategies for the evaluation of cross sections. In particular, the possibility to implement machine learning techniques in combination with the run of massive amount of benchmarks simulation will be discussed.

References:

[1] D. Laghi et al. (2020) "JADE, a new software tool for nuclear fusion data libraries verification & validation". In: *Fusion Engineering and Design* **161** 112075
[2] D. Laghi et al. (2021) "Application of JADE V&V capabilities to the new FENDL v3.2 beta release". In: *Nuclear Fusion* **61** 116073

Physics-Informed Neural Networks for Linear One-Dimensional Diffusion-Advection-Reaction Equations

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Abstract

This work aims to solve seven problems with four different Physics-Informed Machine Learning frameworks and compare the results in terms of accuracy and computational cost. First, we considered the Diffusion-Advection-Reaction Equations, which are second-order linear differential equations with two boundary conditions. The first algorithm is the classic (or standard) Physics-Informed Neural Networks (PINNs). The second one is Physics-Informed Extreme Learning Machine (PIELM). The third architecture is Deep-Theory of Functional Connections (Deep-TFC), a multi-layer NN based on the solution approximation via a constrained expression that always analytically satisfies the constraints. Finally, the last algorithm is the Extreme Theory of Functional Connections X-TFC, which combines TFC and shallow NN with random features.

Direction-Dependent Turning Leads to Anisotropic Diffusion and Persistence

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Abstract

Cells and organisms follow aligned structures in their environment, a process that can generate persistent migration paths. Kinetic transport equations are a popular modelling tool for describing biological movements at the mesoscopic level, yet their formulations usually assume a constant turning rate. Here we relax this simplification, extending to include a turning rate that varies according to the anisotropy of a heterogeneous environment. We extend known methods of parabolic and hyperbolic scaling and apply the results to cell movement on micro-patterned domains also through numerical simulation of the transport model. We show that inclusion of orientation dependence in the turning rate can lead to persistence of motion in an otherwise fully symmetric environment, and generate enhanced diffusion in structured domains.

The state fo the art in biomedical cyclotrons

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Abstract

Cyclotrons are one of the most important sources of radionuclides used in biomedical applications. The production of important radionuclides used in single photon emission tomography techniques such as ^{123}I, ^{67}Ga, ^{201}Tl and ^{111}In has been based for decades on cyclotrons, typically proton machines with an energy up to 30 MeV.
The extraordinary growth of positron emission tomography has led to the development of new models, and to the installation of numerous cyclotrons, typically accelerating proton in the energy range 10 - 20 MeV. These have been used for the production of the main PET radionuclides, namely ^{11}C, ^{13}N, ^{15}O and above all ^{18}F. Recently, their use has been extended to the production of radiometals, like ^{68}Ga, and even to the direct production of ^{99m}Tc. This review presents the main manufacturers and briefly discuss the characteristics of the models they currently offer on the market.
The company IBA has a large portfolio of accelerators. Remaining only in the field of those for the production of radionuclides, we go from 70 MeV of the Cyclone 70, then we have the IKON, the new 30 MeV system, up to 9.2 of the Cyclone KEY; the pivot of the range is the KIUBE, the 18 MeV system which is one of the most modern for the production of PET radionuclides.
GE offers the PETtrace, an extremely successful 16.5 MeV PET cyclotron, easy to operate and maintain; the MINItrace operates a 10 MeV and is typically sold in self shielded configuration, and the GENtrace, at 7.8 MeV completes the offer for entry level production of ^{18}F and ^{11}C.
Advanced Cyclotron Systems Inc (ACSI) produces a full range of variable energy cyclotrons: the TR-19 (12-19MeV), the TR-24 (15-25MeV), the TR-FLEX (12-30 MeV), and the TR-30 (15 -33 MeV).
The Japanese company Sumitomo has a leading market position in Japan and is now marketing essentially the Cypris HM-12 (Protons 12 MeV; Deuterons 6 MeV), and HM-20 (Protons 20 MeV; Deuterons 10 MeV). BEST-ABT pruduces a 7.5 MeV system for small batches production.
There are currently around 1200 radionuclide production cyclotrons in operation worldwide and overall, the market for cyclotrons for the production of radionuclides is a mature sector, with a variety of systems with excellent characteristics able to satisfy different needs terms in of productivity and budget, and to operate in a reliable and safe way from the point of view of radiation protection.

Non-Conforming 3D Model for PWR Control-Rod Movements without Homogenization and Cusping Effect

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Abstract

Enhanced geometrical capabilities were developed to handle accurate model of Pressurized Water Reactor (PWR) within the IDT solver. Based on previous works, the present communication focuses on tri-dimensional models for controls rods. In particular, this work proposes a transport-based method to avoid control-rod cusping effect generated by homogenizations.
Usually, because of axial nature of PWR core, the size of the axial step of the mesh are about 10-20cm long. On the other hand, rods keep moving within the PWR core with a step size of about 1–2 cm along the axial direction. Unavoidably, a control rod cluster may be partially inserted into a set of Cartesian nodes requiring, thus, a heterogeneous representation of cross sections along the z-axis.
As piece-wise distributed cross sections within a node is not allowed in tri-dimensional transport solvers, which are traditionally based on extruded or prismatic geometries. In that case, the heterogeneous node should be homogenized. In recent years, transport-based solvers have been developed to produce high-fidelity calculations of the reactor. Those solvers dealt with control-rod cusping issue by proposing flux-weighting homogenization techniques. However, the simple homogenization generates wiggles in the numerical simulation of the worth, which, theoretically, should be a smooth function of the insertion height of the rod. This phenomenon is the so-called control rod cusping effect (Si, 2006). Since 1980s (Han-Sem, 1984), many methods have been investigated to eliminate it. As an example, Fanning and Palmiotti (1997) developed a heterogeneous Variational Nodal Method (VNM (Palmiotti et al., 1995, Li et al., 2015a)) in PN or SPN framework. In 2003, Smith et al. (2003) developed another heterogeneous VNM. The main idea of this methods is to represent each heterogeneous node by sub-elements within which the cross sections are constants. The spatial and angular moments of the flux are obtained by Galerkin projection of the differential operator over the sub-elements of the node.

In this work, discrete-ordinates Linear Short Characteristics (LSC) are applied to tri-dimensional Heterogeneous Cartesian Cells (HCC) for an accurate pin-by-pin representation of the core. Neither homogenization procedure nor mesh adjustment is needed by taking advantage of the geometrical model. The HCC combines an inner local tridimensional grid with a set of cylinders that represents the rod in its exact shape. The HCC generates a local non-confirming heterogeneous mesh to exactly model the tridimensional details of the geometry.

The new modular pattern allows for a local refinement of axial steps to follow movements of the rods. The planes generated by the axial steps are local to the set of HCCs representing the control-rods. Therefore, they are not prolonged throughout the entire XY cross-section of the core. This avoids mesh adjustments and, consequently, a higher computational cost.

Spatial integrals within HCCs are numerically performed using modular tridimensional ray tracing. The ray tracing technique is establish on the local combinatorial geometry which is composed by the intersection of cylinders with a local XYZ grid. In this manner, a single HCC can be equipped with several local steps to follow with precision the axial displacement of the control rod. The IDT solution algorithm relies on a conformal 3D Cartesian mesh hosting the heterogeneous nodes. In this framework, LSC provides angular-dependent collision-probabilities matrices that explicitly solves the spatial moments of the angular flux within each region of the heterogeneous node. A standard sweeping algorithm solves for the flux distribution by coupling interface angular moments on the boundaries of the HCCs.

Numerical results show that this model eliminates the cusping effect and obtain accurate power distribution with relatively higher efficiency and accuracy.

Angular flux asymptotic expansion applied to discrete-ordinates source iterations for lattice depletion calculations

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Abstract

Fuel lattice simulations for nuclear reactor physics analysis typically involves fuel depletion calculations. Because of flux variations, those simulations generally request high number of media and, thus, of macroscopic effective cross sections. The parameters involved in the discretization of the problem geometry and, thus, affecting the number of depleted media, are:
- the temperature feedback, for the spatial variation of fuel and moderator cross-sections by Doppler effect,
- the self-shielding effect, for spatial variations of multigroup cross sections because of the resonances of the microscopic cross-sections of fuel isotopes.
- the fuel depletion, modelling the spatial distribution of isotopic concentrations within the fuel pins.

In this context, numerical methods based on the integral transport equation, as Collision Probabilities (CP) or Current-Coupling Collision Probabilities (CCCP), suffer severe memory burden as the number of regions and media increases.

This work presents an asymptotic technique that allows for an effective reduction of the memory imprint of discretized coefficients at cost of an increased number of applications of the transport operator. This method is applied to the Heterogeneous Cartesian Cells (HCC) of the transport solver IDT, which solves the neutral-particle transport equation by discrete ordinates.
The spatial representation of the volume sources and of the interface fluxes is up the linear order. The HCC generally represents a physical pin-cell: HCCs sharing the same geometry and having the same set of cross sections share also the same set of coefficients. In depletion calculation, because of the change of the total macroscopic cross section of the media, the HCC discretization would require the construction and the storage of a set of CP coefficients for any HCC composing the geometry. When the number of media grows, IDT performances are hardly affected by the growing of coefficient number, demanding a large amount of memory as well as computational time.

In this work, we will present a practical application of the asymptotic expansion on a 2D UOX assembly simulation with a simulated randomly distributed variation of the fuel and moderator temperatures. Preliminary results show encouraging reductions of about by a factor 10 and without any significate loss of accuracy.

Charge transport in graphene nanoribbons by means of the semiclassical Boltzmann equation

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Abstract

Graphene nanoribbons are considered as one of the most promising ways to design electron devices where the active area is made of graphene. In fact, graphene nanoribbons present a gap between the valence and the conduction bands as in standard semiconductors such as Si or GaAs, at variance with large area graphene which is gapless. The absence of gap limits the use of graphene in field effect transistors (FETs) because there exists a restricted current-off region.
To use graphene nanoribbons as a semiconductor, an accurate analysis of their electron properties is needed. Here, electron transport in graphene nanoribbons is investigated by solving the semiclassical Boltzmann equation. All the electron-phonon scattering mechanisms are included.
Usually the energy dispersion relation is split in subbands and it is related to the shape of the boundary, e.g. armchair or zigzag, and to the width of the ribbon. Here as energy bands we adopt those formulated in [1] which are in good agreement with DFT calculations up to energy of 1 eV, high enough for device applications. The edge effects are described as an additional scattering stemming from the Berry-Mondragon model [2] which is valid in presence of edge disorder.
We simulate the electron transport in GNRs and study the degradation of the mobility due to the confinement and the edge effects. As numerical approach, we adopt both a discontinuous Galerkin method [3] and the direct simulation Monte Carlo. A comparison between results of simulations is performed.

References

[1] M. Bresciani, P. Palestri, D. Esseni, L. Selmi, Simple and efficient modeling of the E-k relationship and low-field mobility in Graphene Nano-Ribbons, Solid-State Electronics, vol. 54, 1015–1021 (2010).
[2] V. K. Dugaev, M. I. Katsnelson, Edge scattering of electrons in graphene: Boltzmann equation approach to the transport in graphene nanoribbons and nanodisks, Physical Review B, vol. 88, 235432 (2013).
[3] G. Nastasi, V.D. Camiola, V. Romano, Direct simulation of charge transport in graphene nanoribbons, Communications in Computational Physics (2021, in press).

Revisiting the learning process in Machine Learning from a partial differential equation point of view: what transport can bring

Gael Poette & Paul Novello & David Lugato
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Abstract

On one hand, Machine Learning (ML) has made a recent come back and has been successfully applied to many physical applications [3,4,5,6]. On another one, its application remains controversial due to its lack of explainability. This work is motivated by both a better understanding of the mechanisms of learning, namely an optimisation process in high dimension in a non-convex context, and the intriguing section of Papanicolaou's famous paper "Asymptotic Analysis of Transport Processes" [1] entitled "learning theory and other examples".
In this talk, we revisit classical ML notions and algorithms under the point of view of the numerician, i.e. the one who is interested in the resolution of partial differential equations (PDEs). We present ML differently, in a way that (we hope) is more adapted to physicists or people with a PDE background. We aim at providing an original and illustrated state-of-the-art of ML optimisers. By a kind of reverse engineering, we explain how the most classical ML algorithms are built. It allows us having a better understanding of their limitations and of how they must be used for efficiency. The basic desired properties of ML algorithms are stated and illustrated. An original (PDE based) framework is suggested, tested and gives interesting satisfactory results. In particular, we highlight and justify an analogy between ML frameworks (such as TensorFlow, PyTorch, SciKitLearn etc.) and the Monte-Carlo (MC) codes used in computational physics: ML frameworks can be viewed as instrumented MC codes solving a parabolic PDE with (well identified) modeling assumptions [2]. Finally, we bridge the gap between transport and diffusion for machine learning, as put forward in [1], and investigate how solving the transport equation instead of the drift-diffusion one (as suggested in [1]) may help us in our ML context. We even design a new transport based learning algorithm and presents few results.

[1] G. C. Papanicolaou. Asymptotic Analysis of Transport Processes. Bulletin of the American Mathematical Society, 81(2), 1975.
[2] G. Poëtte, D. Lugato and P. Novello, An analogy between solving Partial Differential Equations with Monte-Carlo schemes and the Optimisation process in Machine Learning (and few illustrations of its benefits), preprint, 2021.
[3] Gilles Kluth, Kelli Humbird, Brian Spears, Howard Scott, Mehul Patel, Luc Peterson, Joe Koning, Marty Marinakn Laurent Divol and Chris Young. Deep Learning for non-local thermodynamics equilibrium in hydrocodes for ICF. Physics of Plasmas 27, 052707 (2020)
[4] Alexandre Bourriaud, Raphaël Loubère, Rodolphe Turpault. A Priori Neural Networks Versus A Posteriori MOOD Loop: A High Accurate 1D FV Scheme Testing Bed. *Journal of Scientific Computing*, Springer, 2020, 84 (2)
[5] Jonathan Tompson, Kristofer Schlachter, Pablo Sprechmann, Ken Perlin, Accelerating eulerian fluid simulation with convolutional networks, ICML'17: Proceedings of the 34th International Conference on Machine Learning - 70, 2017,3424–3433
[6] Liu Yang, Xuhui Meng, George Em Karniadakis, B-PINNs: Bayesian physics-informed neural networks for forward and inverse PDE problems with noisy data, Journal of Computational Physics, Volume 425, 2021

Building and solving efficient reduced models for the uncertain linear Boltzman equation: applications to neutronics (keff) and photonics

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Abstract

Many physical or economical applications rely on Monte-Carlo (MC) codes to solve *deterministic* partial differential equations (PDEs). This is the case for example for (non-exhaustive list) neutronics and photonics. The Monte-Carlo resolution implies the sampling of the physical variables: $x \in \mathbb{R}^3$ the position, $v \in \mathbb{R}^3$ the velocity and $t \in \mathbb{R}^+$ the time. The simulations are costly but the MC resolution is competitive with respect to other methods due to the high dimensional $(x(3) + v(3) + t(1) = 7)$ *deterministic* problem. The numerical parameter controling the accuracy is N_{MC}, the number of *particles*. The larger N_{MC}, the more accurate the results. The convergence rate obeys the central limit theorem: it is $\mathcal{O}(\frac{1}{\sqrt{N_{MC}}})$.

Obviously, propagating uncertainties (for sensitivity analysis etc.) with respect to different parameters $X \in \mathbb{R}^d$ is of great interest in every of the aforementioned applications (uncertain cross-sections etc.). In fact, in our physical applications, we would like to be able to perform *systematic uncertainty propagations*. As a consequence, we often face a 7+d dimensional problem. Non-intrusive methods are usually applied (use of black box codes). But it demands a high number N of evaluations. In our MC resolution context, each one of them is costly. One accurate run can take several hours on hundreds of processors.

When applying any non-intrusive method to propagate uncertainties through the linear Boltzmann equation solved with an MC code, basically, the physical space (x, t, v) *and* the uncertain space (X) are both explored thanks to two different MC experimental designs. The first one has N_{MC} particles to explore the space of physical variables (x, t, v), the second one has N runs for the space of the uncertain variable X. In this non-intrusive context, the two MC samplings are tensorised in the sense we process $N_{MC} \times N \approx 10^9 - 10^{15}$ particles for an overall $\mathcal{O}(\frac{1}{\sqrt{N_{MC}}})$error. An uncertainty propagation study is consequently costly. The main idea of the present work comes from the fact that MC experimental designs should allow avoiding the tensorisation of the N_{MC} particles and N runs [1,2,3,4]. For this, we sample the whole space relative to (x, t, v, X) within the same MC design. This implies sampling the uncertain parameters X within the code, hence the intrusiveness of the approach. In practice in [1], fast convergence rates have been observed with respect to the polynomial Chaos truncation order P: the method is efficient for the linear [2], nonlinear [4] Boltzman equation and keff computations [3]. The aim of the talk is to present the details of the uncertain MC solver.

[1] G. Poëtte. A gPC-intrusive Monte-Carlo scheme for the resolution of the uncertain linear Boltzmann equation. Journal of Computational Physics, 385:135 – 162, 2019

[2] G. Poëtte. Spectral convergence of the generalized Polynomial Chaos reduced model obtained from the uncertain linear Boltzmann equation. Preprint submitted to Mathematics and Computers in Simulation , 2019.

[3] G. Poëtte and E. Brun. Efficient uncertain k eff computations with the Monte Carlo resolution of generalised Polynomial Chaos Based reduced models. Preprint,November 2020.

[4] G. Poëtte. Efficient uncertainty propagation for photonics: combining Implicit Semi-analog Monte Carlo (ISMC) and Monte Carlo generalised Polynomial Chaos (MC-gPC). Preprint, 2020.

Long-wave oscillations of electrical field for Vlasov--Poisson--Landau equations

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Abstract

The paper is devoted to analytical and numerical study of solutions to the Vlasov-Poisson-Landau kinetic equations (VPLE) for distribution functions with typical length L such that $\varepsilon = r_D/L << 1$, where r_D stands for the Debye radius. It is also assumed that the Knudsen number $Kn = l/L = O(1)$, where l denotes the mean free pass of electrons. We use the standard model of plasma of electrons with a spatially homogeneous neutralizing background of infinitely heavy ions. The initial data is always assumed to be close to neutral. We study an asymptotic behavior of the system for small $\varepsilon > 0$. It is known that the formal limit of VPLE at $\varepsilon = 0$ does not describe a rapidly oscillating part of the electrical field. Our aim is to fill this gap and to study the behavior of the "true" electrical field near this limit. Two classes of initial conditions are considered. In case of standard isotropic in velocities Maxwellian initial conditions, there is almost no damping of these oscillations in the collisionless case. An approximate formula for the electrical field is derived and then confirmed numerically by using a simplified BGK-type model of VPLE. Another class of initial conditions leads to strong oscillations having the amplitude of order $O(1/\varepsilon)$. Numerical solutions of that class are studied for different values of parameters ε and Kn.

Towards a systematic requirement based approach to build a neutronic study platform

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Abstract

Design and safety assessment of nuclear reactors rely on a combination of calculations performed by several simulation tools, each dedicated to a specific ensemble of phenomena, which are later coupled in a multi-physics platform. This procedure is the so-called "calculation chain". For instance, lattice neutronics calculations are meant to provide multi-parameter libraries of few groups cross sections that enable full-core neutronic calculations, which later feed thermal simulations of the fuel rods, which indeed provide feedbacks to neutronic and thermo-hydraulic codes.
Previous generation calculation codes, like SCIENCE v2 currently in production at Framatome,[1] rely mostly on calculation coupled via input and output files. Indeed, recent trends in nuclear industry push towards a more advanced coupling between physics, allowing to perform studies in which the analyst is able to interrogate and modify the state of the calculation core. A modern architecture comprising different software layers dedicated to the underlying numerical methods and to the engineering objects has been already implemented in COCAGNE,[2] the neutronic core code under development by EDF and Framatome.

In the H2020 CAMIVVER project,[3] a task is dedicated to define and implement a multi-parameter neutronic library generator based on the deterministic neutronic code APOLLO3®.[4] APOLLO3® is the successor of the APOLLO2,[5] presently in production at Framatome and EDF.
Calculation codes are often based on the "monolithic approach", in which the solution backend is tightly coupled with the user frontend: the processing is generally based on a first parsing of an input deck to later produce output files. This methodology has several drawbacks, since the analyst cannot perform online branching decisions or cannot reuse some memory structures to perform additional calculations. To overcome these limitations, APOLLO2 provides an internal user language GIBIANE, that allows the analyst to program the calculation backend. However, the GIBIANE is a low-level API, that motivates upper level input generators, as done in APOLLO2-A.[6]
The main difficulty of previous methodologies is that the calculation code may have different client with quite different needs. In this paper, we present a structured way to identify and trace the user needs to define and develop a neutronic calculation platform, employing the system engineering best practices, starting with the identification of use cases and a later generation of system requirements, following the well-known V model.[7][8]
CAMIVVER Work Package 4 aims at providing a calculation platform based on four pillars: flexibility of modeling and analysis options, consistency of requirements specification, innovative algorithm and improved precision, state-of-the art software platform and architecture. We will show how a structured requirement-based approach is capable of better identifying the user and the developer views, allowing a joint collaboration and exchange to overcome the limitation of previous-generator codes.
The specification tree has been therefore identified to let all the actors provide inputs systematically to clearly identify the roles of each component and to let the neutronic calculation code move from a research workbench to an industrial-standard tool. The subsequent breakdown of use case categories allows to link the analyst needs with the backend mechanics.

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APOLLO3® is a registered trademark of the CEA developed under the long-term partnership and support of EDF and Framatome.

References

[1] P. Girieud, I. Daudin, C. Garat, P. Marotte, S. Tarle, S. (2001). "Science version 2: the most recent capabilities of the Framatome 3-D nuclear code package". International Conference on Nuclear Engineering, France
[2] Ansar Calloo, David Couyras, François Févotte, Matthieu Guillo, Coline Brosselard, Bertrand Bouriquet, Alexandre Dubois, Enrico Girardi, Fabrice Hoareau, Marie Fliscounakis, Hadrien Leroyer, Etienne Noblat, Yann Pora, Laurent Plagne, Angélique Ponçot, Nadine Schwartz (2017). "COCAGNE: EDF new neutronic core code for ANDROMÈDE calculation chain". M&C 2017 - International Conference on Mathematics & Computational Methods Applied to Nuclear Science & Engineering
[3] D. Verrier, B. Vezzoni, B. Calgaro, O. Bernard, A. Previti, C. Lafaurie, A. Hashymov, P. Groudev, A. Stefanova, N. Zaharieva, F. Damian, P. Mosca, D. Tomatis, U. Bieder, A. Willien, N. Dos Santos, L. Mercatali, V. H. Sanchez-Espinoza, N. Forgione, S. Paci. "Codes and Methods Improvements for VVER Comprehensive Safety Assessment: The CAMIVVER H2020 Project.", Proceedings of the 2021 28th International Conference on Nuclear Engineering. Volume 2: Nuclear Fuels, Research, and Fuel Cycle; Nuclear Codes and Standards; Thermal-Hydraulics. Virtual, Online. August 4–6, 2021. V002T07A010. ASME.doi:10.1115/ICONE28-64169
[4] D. Schneider, F. Dolci, F. Gabriel, J.-M. Palau, M. Guillo, B. Pothet, P. Archier, K. Ammar, F. Auffret, R. Baron, A.-M. Baudron, P. Bellier, L. Bourhrara, L. Buiron, C. De Saint Jean, J.-M. Do, B. Espinosa, E. Jamelot, V. Jouault, J.-J. Lautard, R. Lenain, J.-C. Le Pallec, L. Lei Mao, E. Masiello, F. Moreau, P. Mosca, M. Muniglia, N. Ordy, V. Pascal, B. Roque, A. Targa, C. Patricot, S. Santandrea, D. Sciannandrone, J.-F. Vidal, I. Zmijarevic (2016). "APOLLO3 CEA/DEN deterministic multi-purpose code for reactor physics analysis." PHYSOR 2016 – Unifying Theory and Experimentsin the 21st Century, May 2016, Sun Valley, USA
[5] R. Sanchez, I. Zmijarevic, M. Coste-Delclaux, E. Masiello, S. Santandrea, E. Martinolli, L. Villate, N. Schwartz, N. Guler (2010). "APOLLO2 year 2010". Nuclear Engineering and Technology, 42. doi:10.5516/NET.2010.42.5.474.
[6] E. Martinolli, T. C. Carter, F. Clement, P. M. Demy, M. Leclere, P. Magat, A. Marquis, V. Marotte, M. Schneider, L. Villatte, J. Marten, S. Misu, S. Thareau (2010). "APOLLO2-A - AREVA's new generation lattice physics code: Methodology and validation.". PHYSOR 2010: Advances in Reactor physics to Power the Nuclear Renaissance, Pittsburgh, PA (USA)
[7] W. Royce (1970). "Managing the Development of Large Software Systems". Proceedings of IEEE WESCON, 26, 1-9. Los Alamitos, CA, USA.
[8] R. Pressman and B. Maxim (2001). "Software Engineering: A Practitioner's Approach". McGraw Hill.

Comparative analysis between fuel assembly calculation capabilities using APOLLO2 and APOLLO3® codes

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Abstract

Performances and safety assessment of nuclear reactors relies today in the so-called two-step approach, where full or piecewise fuel assembly homogenizations are calculated with fine-group deterministic transport calculations to prepare few-group libraries of homogenized cross sections and power distributions, that are later provided to three-dimensional calculation of the whole reactor core.[1] The main advantage of the deterministic approach is to be able to provide fast yet accurate solutions for all the possible combinations of the state parameters characterizing the behavior of the fuel assembly in the reactor core.
This task requires the so-called calculation schemes, i.e. protocols defining solvers and options to construct the final results, striking a balance between discretization precision and physical approximations. Since each application may require different settings, the calculation toolbox should let the advanced developer define different calculation schemes, while giving end-user predefined recipes for the typical applications. For instance, the neutronic response of LWR fuel assemblies can be simulated with the APOLLO2 code system,[2] employing the SHEM energy mesh[3] and the REL2005[4] or ARCADIA[5] schemes. More specifically, the SHEM-MOC, REL2005,[6] and ARCADIA industrial and best estimates[7] schemes have been independently validated for PWR applications.

The H2020 CAMIVVER project[8] aims at establishing calculation methodologies for VVER and PWR assemblies employing the APOLLO3® code system[9]. This paper presents the comparative analysis of APOLLO2 and APOLLO3® calculations for UOX[10], MOX[11], and UOX+Gd[12] benchmark fuel assemblies with and without AIC/B4C control rods. The direct SHEM-MOC like scheme has been adopted. It prescribes a self-shielding step followed by a transport solution and a later homogenization/condensation in the output energy and spatial discretization. Indeed, these computations occur in different geometrical representations, since self-shielding employs the collision probabilities while the transport solution relies on the long characteristics solver. At the same time, the two codes offer quite different interfaces to define geometries: e.g. the windmill meshin APOLLO2[4] has been represented with a circular ring in APOLLO3®. SHEM-MOC[4] options have been reproduced in APOLLO3® as much as possible except the mixture self-shielding, treated instead as isolated isotopes. The state parameters automatically managed in APOLLO2-A[5] have been re-implemented in APOLLO3® employing a Python script looping over the burn-up, fuel temperature, and moderator density. The comparisons of multiplication factors in evolution confirm a good agreement between the two codes, including the possibility to attain the same Gd peak for UOX+Gd assemblies. Relative differences on isotopic compositions do not exceed 1-2%; reaction rate results reach relative differences around 1-1.5% in guide tubes, while for fuel cells they are always under 0.4%.
At last, the flexibility of the two platforms have been evaluated also for parametric studies. The problem chosen is to either normalize or not tracking trajectories in the long characteristic solver.

TRIPOLI-4[14] input decks have been automatically generated by APOLLO3® to provide referencesolutions. APOLLO3® showed a greater flexibility to automatically generate complex Monte Carlo decks while APOLLO2 appeared having a more fine-grained capability to tweak processing.

Acknowledgements
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References

[1] Richard Sanchez (2012). "Prospects in deterministic three-dimensional whole-core transportcalculations". Nuclear Engineering and Technology 44(2). doi:10.5516/NET.01.2012.501
[2] R. Sanchez, I. Zmijarevic, M. Coste-Delclaux, E. Masiello, S. Santandrea, E. Martinolli, L.Villate, N. Schwartz, N. Guler (2010). "APOLLO2 year 2010". Nuclear Engineering and Technology, 42. doi:10.5516/NET.2010.42.5.474.
[3] N. Hfaiedh, A. Santamarina (2005). "Determination of the optimized SHEM mesh for neutrontransport calculation". International Conference on Mathematics and Computation M&C 2005
[4] J. F. Vidal, O. Litaize, D. Bernard, A. Santamarina, C. Vaglio-Gaudard, T. N. Tran (2007). "New Modelling of LWR Assemblies using the APOLLO2 Code Package". Joint InternationalTopical Meeting on Mathematics & Computation and Supercomputing in Nuclear Applications(M&C + SNA 2007)
[5] E. Martinolli, T. C. Carter, F. Clement, P. M. Demy, M. Leclere, P. Magat, A. Marquis, V. Marotte, M. Schneider, L. Villatte, J. Marten, S. Misu, S. Thareau (2010). "APOLLO2-A - AREVA's new generation lattice physics code: Methodology and validation.". PHYSOR 2010:Advances in Reactor physics to Power the Nuclear Renaissance, Pittsburgh, PA (USA)
[6] P. Blaise, J. F. Vidal, A. Santamarina, (2009). "Validation of the REL2005 code package on Gd-poisoned PWR type assemblies through the CAMELEON experimental program". ICAPP2009.
[7] Areva NP (2010). "The ARCADIA® Reactor Analysis System for PWRs MethodologyDescription and Benchmarking Results. Topical Report". https://www.nrc.gov/docs/ML1015/ML101550189.pdf
[8] D. Verrier, B. Vezzoni, B. Calgaro, O. Bernard, A. Previti, C. Lafaurie, A. Hashymov, P. Groudev, A. Stefanova, N. Zaharieva, F. Damian, P. Mosca, D. Tomatis, U. Bieder, A. Willien,
N. Dos Santos, L. Mercatali, V. H. Sanchez-Espinoza, N. Forgione, S. Paci. "Codes and Methods Improvements for VVER Comprehensive Safety Assessment: The CAMIVVER H2020 Project.", Proceedings of the 2021 28th International Conference on Nuclear Engineering. Volume 2: Nuclear Fuels, Research, and Fuel Cycle; Nuclear Codes and Standards; Thermal-Hydraulics. Virtual, Online. August 4–6, 2021. V002T07A010. ASME.doi:10.1115/ICONE28-64169
[9] D. Schneider, F. Dolci, F. Gabriel, J.-M. Palau, M. Guillo, B. Pothet, P. Archier, K. Ammar, F. Auffret, R. Baron, A.-M. Baudron, P. Bellier, L. Bourhrara, L. Buiron, C. De Saint Jean, J.-M. Do, B. Espinosa, E. Jamelot, V. Jouault, J.-J. Lautard, R. Lenain, J.-C. Le Pallec, L. Lei Mao, E.Masiello, F. Moreau, P. Mosca, M. Muniglia, N. Ordy, V. Pascal, B. Roque, A. Targa, C. Patricot, S. Santandrea, D. Sciannandrone, J.-F. Vidal, I. Zmijarevic (2016).

"APOLLO3 CEA/DEN deterministic multi-purpose code for reactor physics analysis." PHYSOR 2016 – Unifying Theory and Experimentsin the 21st Century, May 2016, Sun Valley, USA

[10] Pierre Coppolani, Nathalie Hassenboelher, Jacques Joseph, Jean-François Petetrot, Jean-Pierre Py, Jean-Sébastien Zampa (2004). "La chaudière des réacteurs à eau sous pression". EDPSciences. doi: 10.1051/978-2-7598-0157-2

[11] Akio Yamamoto, Tadashi Ikehara, Takuya Ito, Etsuro Saji (2002). "Benchmark Problem Suite for Reactor Physics Study of LWR Next Generation Fuels". Journal of Nuclear Scienceand Technology, 39:8, 900-912. doi: 10.1080/18811248.2002.9715275

[12] Nam Zin Cho. "Benchmark Problem 1A: MOX Fuel-Loaded Small PWR Core (MOX Fuelwith Zoning)". http://nurapt.kaist.ac.kr/benchmark

[13] X-5 Monte Carlo Team (2003). "MCNP - Version 5, Vol. I: Overview and Theory". LA-UR-03-1987

[14] E. Brun, F. Damian, C.M. Diop, E. Dumonteil, F.X. Hugot, C. Jouanne, Y.K. Lee, F. Malvagi, A. Mazzolo, O. Petit, J.C. Trama, T. Visonneau, A. Zoia (2015). "Tripoli-4®, CEA,EDF and AREVA reference Monte Carlo code". Annals of Nuclear Energy 82, 151-160.

Physics-informed Neural Network with Fourier Features for Radiation Transport in Heterogeneous Media

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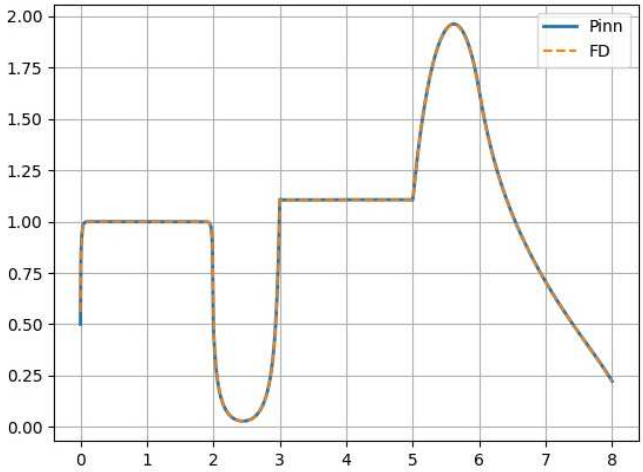
Abstract

Oftentimes, machine-learning (ML) processes are data driven and rely on the acquisition of a large amount of data in order to be trained. In addition, ML processes often lack explainability and purely data-driven methods may not extrapolate well due to observational biases. Therefore, there is a need for incorporating governing laws (e.g., PDEs) to increase the robustness of ML techniques in low-data regime and to enhance their explainability.

In this work, we present a Deep-Learning approach to assimilate the 1D radiation transport in heterogenous media. A deep neural network (4 hidden layers, 8 neurons per layer) is employed to learn the solution of the transport equation. The input layer contains two entries (the independent variables position x and angular direction μ) while the output layer contains only one neuron, for the angular flux $\psi(x, \mu)$. The loss function (or error metric) is formed by the sum of the phase-space residual (i.e., the residual of the transport PDE) at interior phase-space points and the boundary residual (i.e., the boundary conditions). Backpropagation is employed to optimize the neural network hyperparameters (weights, biases, type of activation functions). Adam and limited-memory BFGS are used to solve the optimization problem. The result is a physics-informed neural network architecture, or PiNN, that learned the solution of the transport equation by reducing the interior and boundary residuals, without the need for additional input data. Neural networks, and PiNNs in particular, are knowns to learn more easily diffusive solutions. We observed that tendency for streaming-dominated problems and successfully mitigated it via the use of a Fourier-feature layer past the input layer. The PiNNs we have developed have been tested on a variety of 1D transport problems and compared against finite-difference (FD) solutions. The results are in excellent agreement, as evidenced by the PiNN and FD solution plots for the standard Reed's problem, below, though the solution time for PiNNs is currently significantly larger than that of the FD solver. Extensions of the current work will deal with multi-dimensional transport problems, including local space-angle refinement through the use of PiNNs.



A Hybrid High-Order Low-Order COMET Method for Solving Eigenvalue Neutron Transport Problems

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Abstract

COMET is a hybrid stochastic deterministic coarse-mesh radiation transport method [1] based on the incident flux response expansion theory. It uses a library of surface-to-volume incident flux response expansion coefficients (R_{is}^{m}) to perform iterative transport deterministic sweeps to converge on the solution of the system (problem) of interest made of contiguous coarse-mesh (V_i) such a reactor core. The expansion coefficients (response functions) are precomputed for only the unique coarse-meshes in the system using a continuous-energy stochastic method. The solution is obtained by solving the following (high order) equation iteratively for the phase space partial angular flux moments ($J_{is}^{+,m}$) and the fundamental eigenvalue k.

$$J_{is}^{+,m} = \sum_{s',m'} R_{is's}^{m'm}(k) J_{is'}^{-,m'} \tag{1}$$

In the above equation, the superscripts $\pm$ indicate the outgoing and incoming directions respectively and $R_{is's}^{m'm}$ are the surface (s')-to-surface (s) response expansion coefficients that are calculated using the surface-to-volume response coefficients and the chosen expansion functions as the known boundary condition on the surface of the coarse-mesh (∂V_{is}). The orders of the expansion functions in space and polar and azimuthal angles $(x, y, \vartheta, \varphi)$ are arbitrary. For most problems, depending on their energy (thermal or fast) spectrum, (4,4,2,2) or (2,2,4,4) are sufficient to maintain continuous phase space stochastic accuracy.

In this work, we develop a new high-order low-order method to accelerate the deterministic sweeps (i.e., the solution convergence) in COMET. We begin by introducing the "low-order" equation as written as below.

$$\mathbb{J}_{is}^{+} = \sum_{s'} \mathbb{R}_{is's}(k) \mathbb{J}_{is'}^{-} \tag{2}$$

Here, $\mathbb{J}$ and $\mathbb{R}$ represent the low-order partial current and response functions. We require the total partial current to be preserved by the low-order approximation (i.e., $\mathbb{J}_{is}^{\pm} = J_{is}^{\pm,0}$), i.e.,

$$\mathbb{J}_{is}^{+} = \sum_{s'} \mathbb{R}_{is's} \mathbb{J}_{is'}^{-} = \sum_{s'm'} R_{is's}^{m'0} J_{is'}^{-,m'} \tag{3}$$

One can then derive the following definition for the low-order response functions that preserve the balance of particles on each surface.

$$\mathbb{R}_{is's} = \frac{\sum_{m'} R_{is's}^{m'0} J_{is'}^{-,m'}}{J_{is'}^{-,0}} \tag{4}$$

Note that, this is equivalent to using the exact incoming flux phase space distribution to compute (i.e., collapse) the low-order response functions on-the-fly. Since $J_{is}^{\pm,m}$ and $\mathbb{R}_{is's}$ are not a known a *priori*, they can be iteratively determined.

In the new iterative convergence method, we decompose the response matrix in Eq. (1) into its diagonal/uncollided ($R_{D,is's}^{m'm}$) and off-diagonal/collided ($R_{OD,is's}^{m'm}$) terms/matrices as follows:

$$J_{is}^{+,m} = \sum_{s',m'} J_{is'}^{-,m'} \left(R_{D,is's}^{m'm} + R_{OD,is's}^{m'm} \right) = \sum_{s',m'} J_{is'}^{-,m'} R_{D,is's}^{m'm} + \sum_{s',m'} J_{is'}^{-,m'} R_{OD,is's}^{m'm} \quad (5)$$

$$R_{D,is's}^{m'm} = R_{is's}^{mm} \delta_{m'm} \quad (6)$$

$$R_{OD,is's}^{m'm} = R_{is's}^{m'm} \text{ (for } m' \neq m) \quad (7)$$

The following steps are performed to converge the solution:

1. Use the initial estimate $\mathbb{R}_{is's}(k) = R_{is's}^{00}$(k), where $R_{is's}^{00}$ are the 0th order response functions.
2. Perform low-order eigenvalue calculations (Eq. (2)).
   Perform efficient high-order fixed-source calculations (equivalent to a purely absorbing problem)
   $$J_{is}^{+,m} = \sum_s R_{D,is's}^{mm} J_{is'}^{-,m} + \sum_{m's'} R_{OD,is's}^{m'm} \mathbb{J}_{is'}^{-,m'} \quad (8)$$
3. Use Eq. (4) to update the low-order response functions: $\mathbb{R}$
4. Repeat steps 2-4 until both the low-order and the high-order solutions ($\mathbb{R}, \mathbb{J}$ and J) are converged.

The performance of the new method was tested against direct MCNP [2] Monte Carlo calculations in an advanced AHTR single assembly benchmark problem [3] in uncontrolled and controlled configurations. It was found the difference between the new method's and the MCNP's eigenvalues are 17 pcm and 88 pcm. The average relative differences predicted by the new method are within 3σ of MCNP uncertainties. Each MCNP calculation took about 5 hours on an 84-CPU cluster while the computation time of the low-order method was about 11 seconds on a single CPU. The new method is about 7 times faster than the original high-order COMET.

References:

1. F. Rahnema and D. Zhang, "Continuous energy coarse mesh transport (COMET) method," Annals of Nuclear Energy, 115, pp. 601-610, 2018.
2. X-5 Monte Carlo Team, MCNP—A General Monte Carlo N-Particle Transport Code, Version 5. Los Alamos National Laboratory, 2005.
3. D. Zhang and F. Rahnema, "A stylized 3D Advanced High Temperature Reactor (AHTR) benchmark problem," Annals of Nuclear Energy, 120, pp. 178-185, 2018.

Equilibrium Wigner function for fermions and bosons and quantum hydrodynamical models for charge transport in graphene

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Abstract

The approach based on the Wigner function is considered as a viable model of quantum transport which allows, in analogy with the semiclassical Boltzmann equation, to restore a description in the phase-space. A crucial point is the determination of the Wigner function at the equilibrium which stems from the equilibrium density function. The latter is obtained by a constrained maximization of the entropy whose formulation in a quantum context is a controversial issue. The standard expression due to Von Neumann, although it looks a natural generalization of the classical Boltzmann one, presents two important drawbacks: it is conserved under unitary evolution time operators, and therefore cannot take into account irreversibility; moreover, it does not include neither the Bose nor the Fermi statistics. Recently a diagonal form of the quantum entropy, which incorporates also the correct statistics, has been used in [1]. By adopting such a form of entropy, with an approach based on the Bloch equation, the general condition that must be satisfied by the equilibrium Wigner function is obtained for general energy dispersion relations, both for fermions and bosons.

The Wigner function is then used to get quantum corrected hydrodynamical models for charge transport in graphene [2,3] improving the previous formulations based on the maximum entropy principle in a semiclassical context [4,5].

[1] V. D. Camiola, L. Luca, V. Romano, *Equilibrium Wigner Function for Fermions and Bosons in the Case of a General Energy Dispersion Relation*, Entropy **22**(9), 1023 (2020).

[2] V.D. Camiola, G. Mascali, V. Romano, *Charge Transport in Low Dimensional Semiconductor Structures-The Maximum Entropy Approach*, Springer, 2020.

[3] L. Luca, V. Romano, *Quantum corrected hydrodynamic models for charge transport in graphene*, Ann. Phys. **406**, 30-53 (2019).

[4] V.D. Camiola, V. Romano, *Hydrodynamical model for charge transport in graphene*, J. Stat. Phys. **157**, 114-1137 (2014).

[5] L. Luca, V. Romano, *Comparing linear and nonlinear hydrodynamical models for charge transport in graphene based on the Maximum Entropy Principle*, Int. J. Non-Linear Mech. **104**, 39-58 (2018).

Analysis of the time spectrum of the kinetic transport operator

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Abstract

In the absence of external sources, the solution of the kinetic neutron transport equation with prompt and delayed neutrons in a medium whose properties do not change with time exhibits asymptotic behaviors in $\exp(-\alpha t)$. These modes are independent of earlier changes of the system, in particular of the initial conditions, and a set of so-called alpha eigenvalue equations for the neutron flux and a finite number of precursor concentrations. We have used theoretical results as well as very detailed numerical investigations to analyze the shape of the spectrum and the behavior of the solutions of the alpha eigenvalue problem. We give ample numerical evidence for all the modes predicted from mathematical analysis as well as from physical arguments. Our results are both mathematical and numerical.

The structure of the time spectrum is conditioned by the small contribution of delayed neutron production from radioactive decay and the much greater and faster production from fission. Hence, the operator for the delayed contribution can be considered as a perturbation of the kinetic operator with prompt fission, and the spectrum splits into a prompt spectrum for times or the order of the collision time, $v\Sigma$, and a delayed spectrum with times of the order of the disintegration constants, λp. The entire α spectrum has negative real components with the exception of the dominant eigenvalue which is positive for supercritical problems. The spectrum comprises a point spectrum and a continuum spectrum. The latter is present only in 1D slabs and in infinite 3D domains, as a result of the existence of infinite trajectories, and contains a subset of real, negatives ghost modes which are characterized by null sources and are highly degenerated. Numerical exploration shows that the delayed spectrum contains P denumerable clusters of real eigenvalues with finite multiplicity which accumulate very tightly on the right of each $-\lambda p$ value. Theoretical proof has been given in the literature for simplified problems and we offer also an argument which supports the idea that the full kinetic operator behaves like a compact, self-adjoint operator in the neighborhood of each $-\lambda p$. Each cluster has a dominant simple eigenvalue with a positive flux, but only the greatest dominant eigenvalue has all the concentrations positive.. We introduce a perturbation formulation to establish a new form of the in-hour equation (characterizing point kinetics) and to analyze the so-called flux clustering between the P dominant modes.

For 1D slabs we have written a Python program to construct the matrix for the eigenvalue problem of size NDOF=G R A+Rf P (G=# groups, R=# regions, A=# angles, Rf = # fissile regions and P = # precursors), to directly compute all its eigenvalues. The first summand of NDOF is the dimension of the flux and the second that of the concentrations and correspond, respectively, to the number of eigenvalues in the prompt (the 'continuum') and in the delayed (the P clusters) spectrum. We also present limited results obtained by iterations for a 2D simple problem characteristic of a PWR.

We end discussing a number of open questions?

Benchmarking one group neutron transport equation eigenvalues

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Abstract

The determination of eigenvalues and eigenfunctions of the neutron transport equation is one of the fundamental problems in the physics of nuclear reactors, whose importance is both on the conceptual and on the practical sides. In a series of recent papers [1,2,3] we examined various aspects connected with the P_N expansion of the angular part of the transport equation, related to the nature of the spectra of *k,* α, γ and δ eigenvalues in the complex plane, their relation with the boundary conditions that can be coherently implemented order by order and the even/odd behaviour, a puzzling aspect for a long time, both in one and two groups approaches.

In [3] finally we studied the convergence of the expansion both with respect to the angular representation in Legendre polynomials and to spatial discretization, using and MC simulation as the benchmark to the "exact" result: however this last is available only for the fundamental *k* eigenvalue, so that we miss the possibility to fully validate the (relatively complex) numerical computational methodology: then it would be very useful to have high precision numerical benchmarks for different eigenvalues, also at higher orders. The strategy is then to obtain at least in a relatively simple geometry, e.g. a slab, a very high precision evaluation of the eigenvalues, to be later used as benchmarks to validate the numerical methodology, which then can in principle be applied also to the case of more complex geometries, or other kind of eigenvalues.

One of the possibilities to pursue this goal is to transform the original integro-differential equation into a purely integral one referred only to space variables and then to project the result over an orthogonal set of (spatial) eigenfunction. Carlvik [4] originally employed (again) Legendre polynomials: two kind of difficulties arise within such an approach, the first was connected to the use of floating numbers mathematic leading to numerical instabilities, the second related to the fact that the matrix equation obtained is non linear for anisotropic scattering, leading to the need of iterations.

To overcome these difficulties we made use of the sophisticated abilities of Mathematica™ [5] to use "infinite precision rational arithmetic" with the only limitation of the available memory. This enables us to obtain without particular difficulties the first 50-100 eigenvalues with 20-30 digits of precision, for the case of k eigenvalue, and similar results for other eigenvalues

Bibliography

[1] – N. Abrate, M. Burrone, S. Dulla, P. Ravetto and P. Saracco – Eigenvalue formulations for the P_N approximation to the neutron transport equation, Journ. Comp. Theo. Transp. 49(2020)1-23.

[2] – N. Abrate, S. Dulla, P. Ravetto and P. Saracco – On some features of the eigenvalue problem for the P_N approximation of the neutron transport equation, Ann. Nucl. Energy 163(2021)108477.

[3] – N. Abrate, B.D. Ganapol, S. Dulla, P. Ravetto, P. Saracco, A. Zoia, - Convergence acceleration aspects in the solution of the P_N neutron transport eigenvalue problem, M&C Int. Conference, Raleigh NC, USA, 2021.

[4] – I. Carlvik – Monoenergetic critical parameters and decay constants for small homogeneous spheres and thin homogeneous slabs, Nucl. Sci. Eng. 31(1968)295303.

[5] - Wolfram Research, Inc., Mathematica, Version 12.3.1, Champaign, IL (2021).

Physics-Informed Neural Networks for the Point Kinetics Equations for Nuclear Reactor Dynamics

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Abstract

This work presents a novel approach based on Physics-Informed Neural Networks (PINNs) for the solution of Point Kinetics Equations (PKEs) with temperature feedback. The approach is based on a new framework developed by the authors, which combines PINNs with the Theory of Functional Connections and Extreme Learning Machines in the so-called Extreme Theory of Functional Connections (X-TFC). The accuracy of X-TFC is tested against several published benchmarks (including for non-linear PKEs), showing its accuracy and computational time performance. One of the main advantages of the proposed framework is its flexibility to adapt to a variety of problems with minimal changes in coding and, after the training of the network, in its ability to offer an analytical representation (by Neural Networks) of the solution at any desired time instant outside the initial discretization.

A Novel High-Order Surface Characteristics Scheme for the Neutron Transport Equation on 2D Unstructured Meshes

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Abstract

The method of characteristics (MOC) has become the favourite choice for solving the neutron transport equation at lattice level. Indeed, it relies on a trajectory-based discretization that can treat exactly the streaming term and allows for the use of unstructured and non-conformal 2D meshes. However, a flat approximation (SC) is usually adopted for the source. The resulting scheme exhibits slow spatial convergence and requires a large number of regions for accurate simulations in case of steep flux gradients. The development of higher-order MOC schemes has therefore become of great interest to lower the computational burden of these calculations. For example, a volumetric linear source approximation (VLS) scheme has been recently implemented within the CASMO code.

At CEA Paris-Saclay, a "linear surface" (LS) characteristics scheme was developed and implemented within the TDT lattice solver of the APOLLO3® code. In this technique, volume quantities (neutron flux or emission densities) are reconstructed from a linear interpolation made from surface values. A region-wise rescaling is applied to the interpolation to guarantee the numerical conservation of region averages. The method showed better performances with respect to the SC scheme, but to a certain extent.

In this work, we propose a novel characteristics method that further improves the LS scheme. The goal is to reach higher simulation accuracy or, conversely, to lower computational and memory costs thanks to mesh coarsening (especially in regions with non-evolving materials). In the proposed scheme, the LS region piecewise-constant rescaling factor is allowed to vary in space, thus improving the neutron flux description within the region. Indeed, the higher number of free parameters allows for imposing the conservation of both constant and linear spatial moments of the flux. Compared to the VLS scheme, our new "linear surface-xy" (LSxy) method relies on a surface-based discretization that allows for greater mesh coarsening. Another big difference lies in the adoption of a "differential" approach for the calculation of the flux moments instead of an "integral" one. The former is computationally cheaper and has a lower memory footprint, because it does not require the storage of matrices that are dependent on region, group, and anisotropy-order. Finally, we pay particular attention to the assembly of the streaming term, guaranteeing the robustness of the method even in presence of optically very thin regions.

We assessed the accuracy of the scheme with two test cases: a 3x3 UO_x pattern with an AIC rod (normally employed for V&V purposes of APOLLO3®), and a 17x17 UO_x assembly with B_4C rods. The comparison with Monte Carlo references obtained with the TRIPOLI-4® code shows that the LSxy results (in terms of k_{eff} and reaction rates) are of great accuracy, even in absence of polar sectors in water regions. This proves the superior performances of the proposed method with respect to not only the classic SC or LS schemes but also the VLS one.

Future efforts will focus on accelerating the LSxy iterative solution with the efficient double-P_N synthetic technique, to increase the appeal of the method for industrial calculations.

The Maximum entropy Principle in solid state physics: General approach for dynamic high-Field transport in semiconductor materials and graphene

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Abstract

In the last few decades, the maximum entropy principle (MEP) [1,2] emerged as a powerful method to develop rigorous Extended hydrodynamic (HD) models both in semiclassical [1,2,3,4] and in quantum [5] statistical mechanics. In particular, by starting from microscopic dynamics (band structure, scattering mechanisms, kinetic theory, statistical effects), the MEP managed to provide physical insight into the origin of different terms entering the HD equations, thus leading to a renewed interest in the construction of self-consistent closure relations to investigate charge transport in semiconductors materials [2,3] and graphene [4].
Thus, by using the Maximum Entropy Principle (MEP) [1] we present a general theory to describe high-Field transport phenomena in solid state physics within a dynamical context. In particular, The connections between the conductivity effective mass, the band structure for the hot carriers, with the introduction of a Lorentz factor for the system, and, more generally, the analogies between the monolayer graphene and other physical systems (as the usual semiconductors) in which we have a saturation velocity for the charge carriers are explicitly explained. Will be considered closed Hyperbolic HD system in the framework of Extended Thermodynamics [6] analyzing with critical evaluation these systems (region of Hyperbolicity, band structure, collisional terms, statistics effects) in order to highlight the advantages, the limitations and the future prospects.
In particular we show that, the present HD-MEP method can be fruitfully applied to describe transport properties in graphene with the relevant following advantages: (a) to provide a closed analytical approach and a reduced computational effort with respect to other competitive numerical methods at a kinetic level; (b) to investigate and classify in a systematic way the behavior of the macroscopic moments in dynamic conditions; (c) to distinguish the different regimes of transport by identifying, from an analysis of collisional processes, the dominant scattering mechanisms for a given range of electric Field.

[1] Maximum Entropy and Bayesian Methods, ed. J. Skilling (Kluwer Academic Publishers, 2004).
[2] M. Trovato and L. Reggiani, Riv. Nuovo Cimento 35, 99–266 (2012).
[3] M. Trovato and L. Reggiani, Phys. Rev. B 61, 16667 (2000). M. Trovato and L. Reggiani, Phys. Rev. B 73, 245209 (2006).
[4] M. Trovato, P. Falsaperla , and L. Reggiani, J. Appl. Phys. **125**, 174901 (2019);
[5] M. Trovato and L. Reggiani, Phys. Rev. E 81, 021119 (2010). M. Trovato and L. Reggiani, Phys. Rev. E 84, 061147 (2011). M. Trovato, L. Reggiani, Phys. Rev. Lett. 110, 020404 (2013).
[6] T. Ruggeri and M. Sugiyama, Rational Extended Thermodynamics Beyond the Monatomic Gas (Springer, 2015).

Implicit Monte Carlo with High Order Finite Element Spatial Discretization

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Abstract

In this paper, we will investigate the accuracy and performance of representing all spatially varying quantities, including temperature dependent, and hence spatially dependent opacities, in the Fleck and Cummings Implicit Monte Carlo algorithm, with arbitrarily high order finite element spatial discretizations. To perform such a task, we track particles in the finite element reference space as opposed to standard physical space tracking. Tallies are performed by taking the weak form of the equation they represent and performing a separate "tally" for each basis function with support in the element the particle is passing through. These "tallies" then represent the linear form on the right-hand side of a matrix equation which can be inverted at the end of each Monte Carlo transport step to get the representation of each quantity of interest in a finite element expansion of the chosen basis functions. We will examine spatial convergence order, stochastic error per spatial degree of freedom, and performance metrics for a steady state problem with a known analytical solution. We will then examine several time dependent problems with known analytical or semi-analytical solutions, including several single zone problems and the Su-Olson volume source and Marshak wave problems. Results will be presented for three dimensional cartesian geometries, as well as two dimensional cartesian and cylindrical geometries.

Wigner equations for charge and phonons transport in graphene

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Abstract

Starting from the Von Neumann equation for density operator and by applying the Weyl quantization, Wigner equations for the longitudinal and transversal optical phonons, K-phonons, the longitudinal and transversal acoustic phonons and the Z acoustic phonons are deduced, along with the Wigner equations for charge transport in graphene. With the use of Moyal's calculus and its properties the pseudo-differential operators are expanded up to second order in $\hbar$. We have modelled the phonon-phonon collision operators in a BGK form, describing the relaxation of the Wigner function to a local equilibrium function, depending on a local temperature defined according to [4, 5].

An energy transport model is obtained by using the moment method with closures based on a quantum version of the Maximum Entropy Principle [1, 2, 3].

[1] Barletti, L., Cintolesi, C.: "Derivation of Isothermal Quantum Fluid Equations with Fermi-Dirac and Bose-Einstein Statistics", J Stat Phys 148,353-386 (2012). doi: 10.1007/s10955-012-0535-5
[2] Camiola, V.D., Mascali, G., Romano, V.: "Charge Transport in Low Dimensional Semiconductor Structures, The Maximum Entropy Approach". Springer, (2020).
[3] Luca, L., Romano, V.: "Quantum corrected hydrodynamic models for charge transport in graphene". Annals of Physics, Volume 406, pp. 30-53 (2019) doi:10.1016/j.aop.2019.03.018.
[4] Mascali, G., Romano, V.: "Charge Transport In Graphene Including Thermal Effects". SIAM J. APPL. MATH, Vol. 77, No. 2, pp. 593-613, (2017) Society for Industrial and Applied Mathematics. doi: 10.1137/15M1052573.
[5] Mascali, G., Romano, V.: "A hierarchy of macroscopic models for phonon transport in graphene". Physica A, 548 (2020) 124489. doi: https://doi.org/10.1016/j.physa.2020.12448

Building and solving efficient reduced models for the uncertain linear Boltzman equation: applications to neutronics (keff) and photonics

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Abstract

Many physical or economical applications rely on Monte-Carlo (MC) codes to solve *deterministic* partial differential equations (PDEs). This is the case for example for (non-exhaustive list) neutronics and photonics. The Monte-Carlo resolution implies the sampling of the physical variables: $x \in \mathbb{R}^3$ the position, $v \in \mathbb{R}^3$ the velocity and $t \in \mathbb{R}^+$ the time. The simulations are costly but the MC resolution is competitive with respect to other methods due to the high dimensional $(x(3) + v(3) + t(1) = 7)$ *deterministic* problem. The numerical parameter controling the accuracy is N_{MC}, the number of *particles*. The larger N_{MC}, the more accurate the results. The convergence rate obeys the central limit theorem: it is $\mathcal{O}(\frac{1}{\sqrt{N_{MC}}})$.

Obviously, propagating uncertainties (for sensitivity analysis etc.) with respect to different parameters $X \in \mathbb{R}^d$ is of great interest in every of the aforementioned applications (uncertain cross-sections etc.). In fact, in our physical applications, we would like to be able to perform *systematic uncertainty propagations*. As a consequence, we often face a 7+d dimensional problem. Non-intrusive methods are usually applied (use of black box codes). But it demands a high number N of evaluations. In our MC resolution context, each one of them is costly. One accurate run can take several hours on hundreds of processors.

When applying any non-intrusive method to propagate uncertainties through the linear Boltzmann equation solved with an MC code, basically, the physical space (x, t, v) *and* the uncertain space (X) are both explored thanks to two different MC experimental designs. The first one has N_{MC} particles to explore the space of physical variables (x, t, v), the second one has N runs for the space of the uncertain variable X. In this non-intrusive context, the two MC samplings are tensorised in the sense we process $N_{MC} \times N \approx 10^9 - 10^{15}$ particles for an overall $\mathcal{O}(\frac{1}{\sqrt{N_{MC}}})$error. An uncertainty propagation study is consequently costly. The main idea of the present work comes from the fact that MC experimental designs should allow avoiding the tensorisation of the N_{MC} particles and N runs [1,2,3,4]. For this, we sample the whole space relative to (x, t, v, X) within the same MC design. This implies sampling the uncertain parameters X within the code, hence the intrusiveness of the approach. In practice in [1], fast convergence rates have been observed with respect to the polynomial Chaos truncation order P: the method is efficient for the linear [2], nonlinear [4] Boltzman equation and keff computations [3]. The aim of the talk is to present the details of the uncertain MC solver.

[1] G. Poëtte. A gPC-intrusive Monte-Carlo scheme for the resolution of the uncertain linear Boltzmann equation. Journal of Computational Physics, 385:135 – 162, 2019

[2] G. Poëtte. Spectral convergence of the generalized Polynomial Chaos reduced model obtained from the uncertain linear Boltzmann equation. Preprint submitted to Mathematics and Computers in Simulation , 2019.

[3] G. Poëtte and E. Brun. Efficient uncertain k eff computations with the Monte Carlo resolution of generalised Polynomial Chaos Based reduced models. Preprint,November 2020.

[4] G. Poëtte. Efficient uncertainty propagation for photonics: combining Implicit Semi-analog Monte Carlo (ISMC) and Monte Carlo generalised Polynomial Chaos (MC-gPC). Preprint, 2020.

Kinetic theory study of pressure and EoS in a strongly degenerate Fermi gas

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Abstract

Starting from the Fermi-Dirac distribution function, a strongly degenerate gas of fermions is investigated. Expressions for the density and pressure are given, and the relationship between the two studied to find an Equation of State.