KEN workshop

Report of Contributions

Contribution ID: **1** Type: **not specified**

Welcome coffee

Tuesday, June 10, 2025 9:00 AM (25 minutes)

Contribution ID: **2** Type: **not specified**

Bruno Després (mini course 1): Neural Networks from the viewpoint of Numerical Analysis.

Tuesday, June 10, 2025 9:30 AM (1 hour)

Machine Learning, Neural Networks and Artificial Intelligence are words that one cannot escape from these times. What are some sound mathematical basis for this activity in view of applications to SciML (Scientific Machine Learning) ? This will be the general topic of the course.
- course 1: The compositional structure of NN functions will be analysed within a convenient functional framework inspired by the Murat-Trombetti Theorem. Approximations properties will be reviewed, such as the Cybenko Theorem, the Yarotsky Theorem and some basic analytical formulas.

- course 2: The previous material will be applied to the description of the DeepRitz method for the calculation of a numerical solution to the Poisson equation and to the measurement of the Lipschitz constant of given NN functions in view of stability estimation.

Contribution ID: **3** Type: **not specified**

Bouchra Bensiali (talk 2): A d-dimensional fictitious domain penalization method for Neumann or Robin boundary conditions

Tuesday, June 10, 2025 11:15 AM (45 minutes)

In this talk, we present a d-dimensional extension of a fictitious domain penalization technique we previously proposed for Neumann or Robin boundary conditions. We apply Droniou's approach for non-coercive linear elliptic problems to prove existence and uniqueness of the penalized problem's solution. To establish convergence, we develop a boundary layer approach inspired by the Dirichlet case. However, unlike the Dirichlet setting where estimating remainders is straightforward, convergence here is reduced to the existence of suitable supersolutions of a dual problem. These supersolutions are then constructed as approximate solutions of the dual problem via an additional formal boundary layer approach. The proposed method leads to an advection-dominated problem, requiring numerical methods adapted to singular perturbation problems. We use upwind finite differences to validate the convergence rate and boundary layer thickness, confirming the theoretical predictions. Finally, we explore the potential of this method for problems posed on moving domains, such as those arising in population dynamics under climate change. This talk comprises joint work with Jacques Liandrat, Centrale Méditerranée, I2M.

Contribution ID: **4** Type: **not specified**

Virginie Erhlacher (mini-course 1): Dynamical low-complexity approximations of high-dimensional evolution equations: specific focus on the Schrödinger equation

Wednesday, June 11, 2025 9:00 AM (1 hour)

The aim of this mini-course is to give an overview of various methods to compute dynamical low-complexity approximations of the solution of high-dimensional evolution Partial Differential Equations (PDEs) with a specific focus on the Schro¨dinger equation. In this particular case, the solution of the PDE of interest is in general defined on a very high-dimensional space in the case when the number of electrons in the system is large. As a consequence, traditional numerical methods are doomed to failure because of the curse of dimensionality and specific approaches have to be considered. In particular, it is necessary to rely on the use of some subset of functions which can be represented with a low complexity, and find approximations of the exact solution which belong to such a subset at any time. Several different approaches exist to compute such dynamical low-complexity approximations and the aim of the mini-course is to give an introduction to the most popular methods in this context and give some insight about some recent results.
The first part of the course will be devoted to the presentation of the main subsets of low- complexity functions used in the context of the Schro¨dinger equation such as low-rank tensor formats, polynomial gaussian approximations or neural networks. We will then discuss about the most popular approach used in order to compute dynamical approximations in these subsets, namely the so-called Dirac-Frenkel variational approximation. Lastly, we will discuss about recent results where an alternative variational principle to compute dynamical low-complexity approximations was proposed, relying on a well-conditioned least-square variational formulation of the time-dependent Schr¨odinger equation was proposed. We will discuss about the pros and cons of this new variational principle in comparison with the famous Dirac-Frenkel variational principle.

Contribution ID: **5** Type: **not specified**

Virginie Erhlacher (mini-course 3): Dynamical low-complexity approximations of high-dimensional evolution equations: specific focus on the Schrödinger equation

Thursday, June 12, 2025 9:00 AM (1 hour)

The aim of this mini-course is to give an overview of various methods to compute dynamical low-complexity approximations of the solution of high-dimensional evolution Partial Differential Equations (PDEs) with a specific focus on the Schrödinger equation. In this particular case, the solution of the PDE of interest is in general defined on a very high-dimensional space in the case when the number of electrons in the system is large. As a consequence, traditional numerical methods are doomed to failure because of the curse of dimensionality and specific approaches have to be considered. In particular, it is necessary to rely on the use of some subset of functions which can be represented with a low complexity, and find approximations of the exact solution which belong to such a subset at any time. Several different approaches exist to compute such dynamical low-complexity approximations and the aim of the mini-course is to give an introduction to the most popular methods in this context and give some insight about some recent results.

The first part of the course will be devoted to the presentation of the main subsets of low- complexity functions used in the context of the Schrödinger equation such as low-rank tensor formats, polynomial gaussian approximations or neural networks. We will then discuss about the most popular approach used in order to compute dynamical approximations in these subsets, namely the so-called Dirac-Frenkel variational approximation. Lastly, we will discuss about recent results where an alternative variational principle to compute dynamical low-complexity approximations was proposed, relying on a well-conditioned least-square variational formulation of the time-dependent Schrödinger equation was proposed. We will discuss about the pros and cons of this new variational principle in comparison with the famous Dirac-Frenkel variational principle.

Contribution ID: **6** Type: **not specified**

Bruno Després (mini-course 4): Neural Networks from the viewpoint of Numerical Analysis.

Friday, June 13, 2025 9:00 AM (1 hour)

Machine Learning, Neural Networks and Artificial Intelligence are words that one cannot escape from these times. What are some sound mathematical basis for this activity in view of applications to SciML (Scientific Machine Learning) ? This will be the general topic of the course.
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Contribution ID: **7** Type: **not specified**

Shun Sato (talk 1): On the stability of multi-symplectic diamond schemes

Tuesday, June 10, 2025 10:30 AM (45 minutes)

Evolutionary partial differential equations (PDEs) sometimes have multi-symplectic structures.
For these PDEs, multi-symplectic integrators, numerical methods inheriting the structures, have been widely studied.
In this direction, McLachlan and Wilkins proposed multi-symplectic diamond schemes which use a special mesh called a diamond mesh to fully leverage the local nature of PDEs.
Their method is superior in the sense that it preserves multi-symplecticity, can achieve arbitrarily high-order, and is computationally inexpensive.
However, they applied their method only to simple nonlinear wave equations.
In this talk, we apply their method to a broad class of multi-symplectic PDEs and explore potential stability issues.
This is a joint work with Kaito Sato and Takayasu Matsuo.

Contribution ID: **8** Type: **not specified**

Anxo Biasi (talk 3): Solvable models for energy cascades and condensation via coherent dynamics in Hamiltonian systems

Tuesday, June 10, 2025 2:00 PM (45 minutes)

In this talk, I will present recent results on energy cascades and structure formation in Hamiltonian systems. I will introduce two families of solvable systems that explicitly illustrate the dynamical development of energy cascades and the emergence of large- and small-scale structures. Some solutions represent condensate formation through highly coherent dynamics, while all cascade solutions exhibit power-law spectrum formation in finite time, leading to the blow-up of Sobolev norms and singularities. Such analytic solutions will be compared with numerical simulations, revealing the difficulties numerical methods have to overcome to get accurate descriptions of blow-up and weak turbulence.

Contribution ID: **9** Type: **not specified**

Francis Filbet (talk 4): A structure and asymptotic preserving scheme for the quasi-neutral limit of the Vlasov-Poisson system

Tuesday, June 10, 2025 2:45 PM (45 minutes)

We propose a numerical method for the Vlasov-Poisson system which is asymptotically consistent and stable in the quasi-neutral limit, that is, when the Debye length is small compared to the scale of the domain. The Vlasov-Poisson system is written as an hyperbolic system thanks to a spectral decomposition in the basis of Hermite functions with respect to the velocity variable, then a structure preserving finite volume scheme for the space variable is designed. On the one hand, we show that the Hermite formulation is adequate to study the quasi-neutral limit and get error estimates between the solution to the Vlasov-Poisson system and its asymptotic limit. On the other hand, we apply a numerical scheme, inspired by the previous work, to recover a consistent approximation of the quasi-neutral limit. Finally, we perform substantial numerical simulations to illustrate the efficiency of this approach for a large variety of regimes and to highlight its robustness (conditional stability, asymptotic preserving properties).

Contribution ID: **10** Type: **not specified**

Karolina Kropielnicka (talk 5): Second-Order Time-Splitting Hermite Spectral Method for Nonlinear Schrödinger Equations with Time-Dependent Potential

Tuesday, June 10, 2025 4:00 PM (45 minutes)

In this talk we will be concerned with the Nonlinear Schrödinger Equations with Time-Dependent Potential. We will propose a new numerical method based on splitting in time and spectral method in space. Second order splitting will be obtained via linearisation combined with iterated Duhamel formula. In spectral discretization we will employ the basis of Hermite functions, for which we will present the exact, analytic expression of solution to the free Schrödinger equation.

Contribution ID: **11** Type: **not specified**

Takayasu Matsuo (talk 6): A new convergence estimate of a energy-preserving scheme for the KdV equation

Wednesday, June 11, 2025 10:30 AM (45 minutes)

In this talk, we consider an energy-preserving finite difference scheme for the KdV equation (Furihata, 1996). The scheme preserves the cubic energy function, and has been empirically known that it works better than (L2)norm-preserving schemes. However, since the cubic energy function by itself is not useful in the mathematical analysis of numerical schemes, the convergence estimate of the scheme has been left open until now (in contrast to the norm-preserving cases, where various results are known.)
Recently, we devised a new convergence estimate argument that successfully gives the desired estimate. The argument is constructed in an inductive way, and can be applied to the cases where useful a priori estimates on the solution (such as in L2 or sup) are hard to obtain. It can be applied to other energy-preserving schemes for the generalized KdV or the Ostrovsky equation.

Contribution ID: **12** Type: **not specified**

Lukas Einkemmer (talk 7): Higher-order dynamical low-rank methods

Wednesday, June 11, 2025 11:15 AM (45 minutes)

Dynamical low-rank algorithms have developed into an efficient way to solve high-dimensional problems ranging from plasma physics to quantum mechanics. Those methods are attractive because they reduce a high-dimensional problem into a set of lower-dimensional equations and can thus overcome the curse of dimensionality. This, for example, enables 6D Vlasov simulation on a desktop computer that otherwise would require large supercomputers. Mathematically, dynamical low-rank methods project the true dynamics onto a low-rank manifold (the approximation space). The most common approach to do this robustly is the projector splitting integrator. While composition can be used to raise this to second or higher order, there is currently no rigorous proof available that shows that the resulting scheme is second-order accurate (although this is usually observed in numerical experiments). More recently, a class of so-called (augmented) basis update & Galerkin (BUG) schemes have been introduced. These are, for example, commonly used as the building block for structure-preserving dynamical low-rank schemes. However, the literature on such methods has focused on first-order and explicit methods. In this talk, we present our recent work that allows the construction of higher-order BUG type integrators. In particular, we will show that these integrators are provably second-order accurate. We also show that implicit variants of such methods can be constructed, which e.g. for step and truncate type low-rank algorithms is much more difficult. The resulting implicit schemes have the added benefit that the linear systems that need to be solved are much smaller than for the original problem, while still maintaining desirable properties such as unconditional stability.

Contribution ID: **13** Type: **not specified**

Nicola Guglielmi (talk 8): A fast and memoryless numerical method for solving fractional differential equations

Wednesday, June 11, 2025 2:00 PM (45 minutes)

The numerical solution of implicit and stiff differential equations by implicit numerical integrators has been largely investigated and there exist many excellent efficient codes available in the scientific community, as Radau5 (based on a Runge-Kutta collocation method at Radau points) and Dassl, based on backward differentiation formulas, among the others. When solving fractional ordinary differential equations (ODEs), the derivative operator is replaced by a non-local one and the fractional ODE is reformulated as a Volterra integral equation, to which these codes cannot be directly applied.
This talk proposes a methodology which makes it possible to make use of such codes. In particular it presents an algorithm for the construction of an approximation of the fractional kernel by a sum of exponential functions, and it shows how the arising linear systems in a stiff time integrator can be solved efficiently. It is explained how the code Radau5 can be used for solving fractional differential equations. Numerical experiments, on both fractional ODEs and 1D PDEs, illustrate the accuracy and the efficiency of the proposed method. Driver examples are publicly available from the homepages of the authors.

Contribution ID: **14** Type: **not specified**

Jingwei Hu (talk 9): An explicit energy-conserving particle method for the Vlasov-Fokker-Planck equation

Wednesday, June 11, 2025 2:45 PM (45 minutes)

We present an explicit particle method for the Vlasov-Fokker-Planck equation that conserves energy at the fully discrete level. The method features two key components: a conservative particle discretization for the nonlinear Fokker-Planck operator (also known as the Lenard-Bernstein or Dougherty operator), and an explicit time integrator that ensures energy conservation through an accuracy-justifiable correction. We validate the scheme on several plasma benchmarks, demonstrating its effectiveness. This work is in collaboration with Lee Ricketson and Jiyoung Yoo.

Contribution ID: **15** Type: **not specified**

Christian Klein (talk 10): Numerical study of fractional nonlinear Schrödinger equations

Tuesday, June 10, 2025 4:45 PM (45 minutes)

A numerical study of solutions to fractional nonlinear Schrödinger (fNLS) equations is presented. We discuss efficient numerical algorithms to compute fractional derivatives. For the focusing fNLS equation, solitons are constructed numerically and their stability is explored. The possibility of a blow-up of solutions to fNLS for smooth initial data is discussed.

Contribution ID: **16** Type: **not specified**

Yuto Miyatake (talk 11): A posteriori and statistical estimation of discretization errors in the numerical solution of evolution equations

Thursday, June 12, 2025 10:30 AM (45 minutes)

In inverse problems and data assimilation, various sources of uncertainty arise. Among them, discretization errors in evolution equations can be significant and should sometimes be treated as a major source of uncertainty to be quantified.

In this talk, we present a posteriori and statistical approaches to estimating such errors. The key idea is to model the discretization error as a random variable and to impose prior information on its distribution. We then estimate statistical quantities such as the variance using numerical solutions and noisy observations of the state variables.

In particular, we introduce discretization error quantification methods based on isotonic regression, a statistical technique for fitting a non-decreasing real-valued function to (typically one-dimensional) data.
We demonstrate efficient algorithms whose computational cost is typically negligible compared to that of solving the overall inverse problem.

Contribution ID: **17** Type: **not specified**

Sheehan Olver (talk 12): Parallelising PDEs using Representation Theory

Thursday, June 12, 2025 11:15 AM (45 minutes)

If a partial differential operator commutes with a symmetry group (permutations, rotations, reflections, etc.) then it can be decoupled by discretising with a so-called symmetry-adapted basis built from irreducible representations, the basic building blocks of representation theory. In this talk we explore this phenomena using symmetry-adapted multivariate orthogonal polynomials to discretise Schrödinger equations with potentials invariant under permutations or the octohedral symmetry group for the cube. To do this systematically we introduce a new algorithm for decomposing representations into irreducibles built on numerical linear algebra.

Contribution ID: **18** Type: **not specified**

Ingrid Lacroix-Violet (talk 13): Linearly implicit numerical methods for semilinear evolution PDEs

Thursday, June 12, 2025 2:00 PM (45 minutes)

In this talk, I will present a new class of numerical methods for the time integration of evolution equations. The systematic design of these methods mixes the Runge-Kutta collocation formalism with collocation techniques in such a way that the methods are linearly implicit and have high order. The fact that these methods are implicit allows to avoid CFL conditions when the large systems to integrate come from the space discretization of evolution PDEs. Moreover, these methods are expected to be efficient since they only require to solve one linear system of equations at each time step, and efficient techniques from the literature can be used to do so. After the introduction of the methods, I will set suitable definitions of consistency and stability for these methods, prove their convergence and order on the ODE case and finally I will present some numerical simulations.

Contribution ID: **19** Type: **not specified**

Luis Chacon (talk 14): Exact local conservation of energy in fully implicit PIC algorithms

Thursday, June 12, 2025 2:45 PM (45 minutes)

Abstract: We consider the issue of strict, fully discrete local energy conservation for a whole class of fully implicit local-charge- and global-energy-conserving particle-in-cell (PIC) algorithms. Earlier studies [1-3] demonstrated these algorithms feature strict global energy conservation. However, whether a local energy conservation theorem exists (in which the local energy update is governed by a flux balance equation at every mesh cell) for these schemes is unclear. In this study, we show that a local energy conservation theorem indeed exists [4]. We begin our analysis with the 1D electrostatic PIC model without orbit-averaging, and then generalize our conclusions to account for orbit averaging, multiple dimensions, and electromagnetic models (Darwin). In all cases, a temporally, spatially, and particle-discrete local energy conservation theorem is shown to exist, proving that these formulations (as originally proposed in the literature), in addition to being locally charge conserving, are strictly locally energy conserving as well. In contrast to earlier proofs of local conservation in the literature [5], which only considered continuum time, our result is valid for the fully implicit time-discrete version of all models, including important features such as orbit averaging. We demonstrate the local- energy-conservation property numerically with a paradigmatic numerical example.

REFERENCES

[1] G. Chen, L. Chacón, and D. C. Barnes, "An energy-and charge-conserving, implicit, electrostatic particle-in-cell algorithm,"Journal of Computational Physics, vol. 230, no. 18, pp. 7018-7036, 2011.

[2] G. Chen, and L. Chacon, "A multi-dimensional, energy-and charge-conserving, nonlinearly implicit, electromagnetic Vlasov–Darwin particle-in-cell algorithm,"Computer Physics Communications, vol. 197, pp. 73-87, 2015.

[3] G. Chen, and L. Chacón, "An energy-and charge-conserving, nonlinearly implicit, electromagnetic 1D-3V Vlasov–Darwin particle-in-cell algorithm,"Computer Physics Communications, vol. 185, no. 10, pp. 2391-2402, 2014.

[4] L. Chacon, and G. Chen, "Exact local conservation of energy in fully implicit PIC algorithms," arXiv preprint arXiv:2410.16530, 2024.

[5] J. Xiao, H. Qin, J. Liu et al., "Local energy conservation law for a spatially-discretized Hamiltonian Vlasov-Maxwell system,"Physics of Plasmas, vol. 24, no. 6, 2017.

Contribution ID: **20** Type: **not specified**

Ansgar Jungel (talk 15): Structure-preserving finite-volume methods for cross-diffusion systems and discrete chain rules

Thursday, June 12, 2025 4:00 PM (45 minutes)

Many thermodynamic mixture and biological multicomponent models can be described by cross-diffusion systems. Although the diffusion matrices are generally neither symmetric and nor positive definite, the systems often possess an entropy (or free energy) structure. We aim to "translate" this entropy structure to fully discrete finite-volume discretizations. The main difficulty is to adapt the nonlinear chain rule to the discrete level.
In this talk, we present two strategies to define a discrete chain rule, assuming either that the entropy is the sum of individual entropies or that the entropy describes volume-filling models. Both strategies use suitable mean formulas, based on the mean-value theorem and the convexity of the entropy functional and work for the implicit Euler scheme. This leads to convergent and structure-preserving finite-volume schemes. Examples include models for segregating populations and Maxwell-Stefan systems for gas mixtures. Extensions to higher-order time approximations are discussed too.

Contribution ID: **21** Type: **not specified**

Fernando Casas (talk 17): The phenomenon of resonances in splitting methods applied to unitary problems

Friday, June 13, 2025 10:30 AM (45 minutes)

Abstract:
There is ample numerical evidente that splitting methods, when applied to the time integration of the (semi-discretized) Schrödinger equation, exhibit numerical resonances at specific values h_r of the time step-size: for these values h_r the errors in the solution and in the energy show a peak. E. Faou has analyzed in detail this phenomenon using backward error analysis techniques, and in particular has shown that resonances are closely related with the non-existence of a modified Hamiltonian.

In this talk, we introduce an alternative approach to explain the origin of these resonances and the non-existence of a modified equation when $h = h_r$ in the finite-dimensional setting. We also describe how the errors in the solution and in energy grow over time at resonance values of the time-step.

This is an ongoing work in collaboration with Sergio Blanes (Valencia), Ander Murua (San Sebasti\'an), and Mechthild Thalhammer (Innsbruck).

Contribution ID: **22** Type: **not specified**

Marianne Bessemoulin-Chatard (talk 18): Discrete hypocoercivity for a nonlinear kinetic reaction model

Friday, June 13, 2025 11:15 AM (45 minutes)

In this talk, I construct and analyze the decay to equilibrium of a finite volume scheme for a 1D nonlinear kinetic relaxation model describing a recombination-generation reaction of two species, proposed in [Neumann, Schmeiser, KRM 2016]. The study is based on the adaptation of the L^2 hypocoercivity method of [Dolbeault, Mouhot, Schmeiser, Trans. Amer. Math. Soc. 2015] for the discretization of the linearized problem. Then, we establish a local result for the discrete nonlinear system. As in the continuous framework, this requires maximum principle estimates, which necessitates the use of monotone numerical fluxes.
This is a joint work with Tino Laidin (Univ. Lille) and Thomas Rey (Univ. Nice).

Contribution ID: **23** Type: **not specified**

Lunch

Tuesday, June 10, 2025 12:00 PM (2 hours)

Contribution ID: **24** Type: **not specified**

Lunch

Wednesday, June 11, 2025 12:00 PM (2 hours)

Contribution ID: **25** Type: **not specified**

Coffee break

Tuesday, June 10, 2025 3:30 PM (30 minutes)

Contribution ID: **26** Type: **not specified**

Lunch

Thursday, June 12, 2025 12:00 PM (2 hours)

Contribution ID: **27** Type: **not specified**

Lunch

Friday, June 13, 2025 12:00 PM (2 hours)

Contribution ID: **28** Type: **not specified**

Coffee break

Wednesday, June 11, 2025 10:00 AM (30 minutes)

Contribution ID: **29** Type: **not specified**

Coffee break

Wednesday, June 11, 2025 3:30 PM (30 minutes)

Contribution ID: **30** Type: **not specified**

Coffee break

Thursday, June 12, 2025 10:00 AM (30 minutes)

Contribution ID: **31** Type: **not specified**

Coffee break

Thursday, June 12, 2025 3:30 PM (30 minutes)

Contribution ID: **32** Type: **not specified**

Coffee break

Friday, June 13, 2025 10:00 AM (30 minutes)

Contribution ID: **33** Type: **not specified**

Coffee break

Contribution ID: **34** Type: **not specified**

Coffee break

Contribution ID: **36** Type: **not specified**

Chengwei Fan (Talk 16): Long-time Error Estimates of Low-Regularity Integrators for Nonlinear Schrödinger Equations

Wednesday, June 11, 2025 4:00 PM (45 minutes)

We investigate the long-time behavior of a resonance-based low-regularity integrator for the cubic nonlinear Schrödinger equation (NLS). Specifically, we analyze the cubic NLS with a weak nonlinearity characterized by a dimensionless parameter $\varepsilon \in (0, 1]$. Through rescaling, this equation is equivalent to the NLS with small initial data. We provide rigorous error estimates for rough initial data $\phi \in H^1$, valid up to times of order O(ε^−α), where α can be chosen up to 4 in one dimension and arbitrarily large in two dimensions.
Notably, in dimension three—and also in dimension two for initial data in the weighted space Σ—we establish uniform-in-time estimates with the help of scattering theory. These results highlight the capability of low-regularity integrators to accurately capture the long-time dynamics of weakly nonlinear dispersive equations with low regularity initial data.

Contribution ID: **37** Type: **not specified**

Welcome

Tuesday, June 10, 2025 9:25 AM (5 minutes)

Contribution ID: **38** Type: **not specified**

Welcome cocktail

Tuesday, June 10, 2025 5:30 PM (1h 30m)