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Computational challenges in high-energy astrophysics

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Summary. — Supercomputers and grid networks are the basic instruments to elaborate and test physical models involving complex astrophysical phenomena. In this review some aspects of the field of high-energy astrophysics are illustrated that require large-scale computations due to the nonlinearities of the physical processes involved. They aim to understand fast dynamical phenomena, like stellar collapses, accretion onto black holes, launching and propagation of relativistic jets; high-energy phenomena involve a strong link between dynamics and microphysics and require a nonequilibrium treatment. A crucial point remains the validation of codes in regimes that are outside laboratory tests.

1. – Introduction

Computer simulations are used in theoretical astrophysics to investigate complex nonlinear problems connecting macro- and micro-scale physical phenomena. Both highperformance and grid computing facilities are powerful tools that have brought unprecedented advances in the field. In this brief review I illustrate examples of high-performance computations developed in recent years to tackle high-energy phenomena. These problems typically require the solution of systems of hyperbolic partial differential equations in both space and time variables covering a large set of scales. Therefore numerical computations require large domains sampled at high resolution with long times of evolution to capture the dynamical details especially around discontinuities and shocks.

Finite-difference codes such as ZEUS [1, 2] or NIRVANA [3] evolved from early experiments at the beginning of the 1960s. However more accurate and robust methods were shown to be necessary to satisfy conservation properties. For this high-resolution shock capturing schemes (HRSC) were developed to investigate fluid dynamics in highly nonlinear regimes. The great advantage of these schemes is their ability to model strongly

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supersonic flows while maintaining robustness and stability. The basic algorithms are based on a conservative formulation of the fluid equations and a proper upwind integration through an approximate or exact solution of the Riemann problem, which yields the decay of discontinuities at the interface of grid cells. This approach was introduced in a pioneering work by Godunov [4].

HRSC codes are designed to integrate the fluid equations in conservative form:

(1)
$$\frac{\partial \mathbf{U}}{\partial t} = -\nabla \cdot \mathbf{T}(\mathbf{U}) + \mathbf{S}(\mathbf{U}),$$

where **U** denotes a vector physical quantity, $\mathbf{T}(\mathbf{U})$ a rank-2 tensor flux of this quantity and $\mathbf{S}(\mathbf{U})$ a vector source term. The integration is performed through the shock-capturing scheme using the finite-volume formalism in which volume averages evolve in time. The volume-averaged quantities **U** are mapped into primitive quantities **V** chosen in a way to allow to control physical constraints (positive pressure and density, subluminal speeds, etc.). Left and right states at grid cell edges are constructed by interpolation inside cells; then the Riemann problem is solved to calculate the numerical flux function **F** at interfaces. Finally the solution is advanced in time. The integration algorithm is independent of the physical content of the equation considered; the physics is contained in the specific forms of $\mathbf{T}(\mathbf{U})$ and $\mathbf{S}(\mathbf{U})$.

Shock-capturing schemes are at present the basic technique in recently developed high-resolution codes, as for instance FLASH for reactive hydrodynamics with relativistic and magnetohydrodynamic modules [5], GENESIS for special relativistic hydrodynamics [6], VAC versatile advection code [7], the new NIRVANA [8] and PLUTO with multi-algorithm modular capabilities [9].

As already pointed out, in astrophysical problems large space domains must be used and their evolution must be followed over long time scales; in addition high resolution is needed in order to simulate nonlinear physical effects at the macroscopic level. For this reason these codes must be parallelized through domain decomposition; grid adaptation is also implemented. Adaptive mesh refinement (AMR) modules are often used to maximize the integration efficiency.

In the following I shall give some examples of recent simulations in the astrophysics of active galactic nuclei to show the contribution of numerical methods in addressing complex systems and at the same time to illustrate their limits.

2. – Magnetohydrodynamics of active galactic nuclei (AGN)

The basic scenario supported by observations suggests that AGNs are powered by a compact object, most likely a black hole, accreting matter and liberating large amounts of gravitational energy, up to $42\% mc^2$ per particle of mass m falling toward the gravitational horizon. The liberated energy contributes to the radiation emission over the entire electromagnetic spectrum including X- and γ -rays and to supersonic outflows under the form of relativistic winds or collimated jets. Accretion disks have been directly observed in a few cases; in particular we mention the case of M87, where optical spectroscopy has allowed to measure the rotation curve of matter around the central nucleus. The study of accretion inflows and emergence of jets from accretion funnels with an evaluation of their power and energy dissipation at various distances from the nucleus represents a challenging problem for MHD fluid dynamics.

2[•]1. Accretion disks. – In the original model of accretion disks Shakura and Sunyaev [10] looked for a stationary solution in which matter accretes in near-Keplerian conditions liberating the gravitational energy necessary for radiation emission. The crucial physical element is the dissipation process that allows the disk matter to lose angular momentum by falling into the gravitational well and at the same time heats the disk. The physical origin of the dissipation remained unclear for many years, until Balbus and Hawley [11] noted that the stability of near-Keplerian disks could be dramatically altered by the presence of magnetic fields. The resulting instability, known as the Magneto-Rotational Instability (MRI), can lead to the exponential growth of infinitesimal perturbations towards a turbulent state. Numerous studies have been published on the nonlinear evolution of the MRI directed towards understanding the saturation process and the characteristics of the emergent turbulent state. In particular Goodman and Xu [12] proved that the MRI reaches the so-called *channel structure* corresponding to axisymmetric motions with no radial dependence, a sinusoidal variation in the vertical direction, and a growth rate that depends on the angle between the velocity and the azimuthal direction. As the amplitude grows, the channel flows is affected by secondary parasitic instabilities, possibly identified with Kelvin-Helmholtz and tearing modes instabilities.

A numerical study of the MRI is needed to evaluate its efficiency in the nonlinear regime. Global 3D MHD simulations have been performed, using relatively low-resolution, short time scales of integration and standard finite-difference (non-shock-capturing) method of integration [13,14]. Apparently the channel solution is not reached in these simulations, but a highly turbulent structure forms. However, the numerical simulations were for very low Reynolds numbers and did not allow a firm conclusion on the characteristics of the turbulent state. Also integration time are relatively short and do not show whether a stationary state is reached.

The alternative approach is based on the local shearing-box approximation in which a small periodic region of the disk is simulated. The method employs a local expansion of the fluid equations in a small region co-rotating with the disk at some fiducial radius R_0 [15]. If the size of the box is sufficiently small, curvature terms can be neglected and a local system of Cartesian coordinates centered around R_0 may be adopted. The advantage of this local approach is the possibility of reaching much higher resolutions and of following the long-term evolution of the MRI instability, towards the formation of the channel flow structure and its saturation towards a turbulent state. Bodo *et al.* have performed a series of 3D, compressible, isothermal simulations, always in the shearing box approximation with different box sizes and aspect ratios using the PLUTO code [16].

In fig. 1 the different behaviour for different aspect ratios of the shearing box is shown. While for aspect ratio 1 an intermittent behaviour appears in which channel flows amplify and then suddenly disappear, for aspect ratio 4 MRI develops towards a stationary turbulent state without the appearance of channel solutions. The important point is that the transport efficiency (viscosity) is on the average overestimated in the cases with aspect ratio 1. It is apparent that studies of turbulence driven by the MRI should be conducted in shearing boxes sufficiently large to allow the solution to develop naturally.

2[•]2. Jets. – Collimated relativistic jets are a natural outcome from magnetized accretion disks, and they are observed in connection with AGNs [17]. Jet acceleration is produced by electrodynamic forces: the interaction between an accretion disk and the magnetic field which threads it is modeled within a resistive MHD framework. High-resolution



Fig. 1. – Time histories of the Maxwell stresses averaged over the computational box and normalized to the pressure. The two panels correspond to cases with aspect ratio 1 and 4. Time is in units of the rotation time.

simulations have been performed by Zanni *et al.* [18] using a modified version of the MHD module provided with the code FLASH [5] with Adaptive Mesh Refinement (AMR). This acceleration phase of jets from disks is discussed in these Proceedings by Tzeferacos [19]. Instead here we illustrate simulations of the propagation phase of jets in the interstellar and intergalactic medium. Observations indicate that most extragalactic jets associated with AGNs move at relativistic speed up to 100 pc–1 kpc scales from the nucleus. At larger distances, reflecting the Fanaroff-Riley radio source classification, we observe an abrupt deceleration in FR-I jets while relativistic motions persist up to Mpc scale in FR-II.

These data can be interpreted by external medium entrainment through shear instabilities, namely Kelvin-Helmholtz instabilities. The nonlinear development of velocity shear or Kelvin-Helmholtz instabilities leads to an exchange of mass, momentum and energy between the jet and the surrounding medium [20]. Numerical simulations of propagating light jets have been performed by Rossi *et al.* in 3D hydrodynamics [21]. Jet inflows are represented by a three-parameter family characterized by the beam Lorentz factor γ_b , Mach number $M = v_b/c_s$ and the ambient-to-beam density contrast η as seen in the observer's frame. Ambient medium is given by $\rho_a = \eta/\gamma_b$. The beam is initially pressure-matched and at the jet inlet the transverse velocities are perturbed introducing pinching, helical and fluting modes with phases randomly chosen. The amplitude of the perturbation corresponds to a fractional change in the bulk Lorentz factor. Outside the inlet region symmetric boundary conditions (emulating a counter-jet) are imposed, whereas the flow can freely leave the domain throughout the remaining boundaries. Integration has been performed using the code PLUTO.

The entrainment process between the jet beam and the cocoon is promoted by the development of Kelvin-Helmholtz instabilities at the beam interface. The entrained material is composed of jet backflowing material mixed with the shocked ambient medium through the contact discontinuity. Keeping fixed the value of the Lorentz factor $\gamma = 10$, the Mach number M and density ratio $\eta = \rho_{\text{ext}}/\rho_{\text{jet}}$ are varied. The process is quite complex and depends on many different factors, the beahavior of KHI being the most relevant. In fig. 2 results are represented for three cases: case A) M = 3, $\eta = 10^2$, case B) M = 3, $\eta = 10^4$, case C) M = 30, $\eta = 10^2$. They show 2D cuts in the *xy*-plane (at z = 0) of the density and Lorentz factors. From the density panels, one can note that in both case A) and C) the jet seems to be weakly affected by the perturbation growth. This is



Fig. 2. – Two-dimensional longitudinal cut in the xy-plane of the density distribution for case A) at t = 240 (top-left panel), case B) at t = 760 (central-left panel) and case C) at t = 150 (bottom-left panel), and Lorentz γ distribution in the central part of the domain, not in scale (the corresponding right panels).

not the situation for case B), where the beam structure is heavily modified by the growth of disturbances after it has reached ~ 20 jet radii. Still, a well-collimated high-velocity component along the axis can be recognized. The distributions of the Lorentz factor (right panels) indicate that the perturbation slightly affects the system in case A) after ~ 100 radii, leaves the jet almost unchanged in case C), and strongly influences the propagation after ~ 20 radii for case B), where the maximum value of γ has reduced approximately to half of its initial value.

In conclusion, in this strongly underdense case, the jet acquires a velocity structure in which the inner core maintains a highly relativistic velocity and is surrounded by material that has been slowed down by the interaction with the ambient medium. A structure of this type (called "spine-layer") has been suggested as an explanation of some observational properties of FR-I radio sources and their beamed counterparts (BL Lac objects).

3. - Conclusions: Code validation and experiments

A crucial, still not always appreciated, issue in the use of numerical codes for modeling astrophysical phenomena is that the typical physical conditions occurring in astrophysical plasmas are very different from those that can be reproduced in numerical simulations. These can probe a very small portion of the astrophysical parameter space (Reynolds number, magnetic Reynolds number, Prandtl number, etc.) for their inherent limitations in resolution, space and time scales. However simulations can examine physical processes in the parameter space that pertains to laboratory experiments. The simulation of nonlinear phenomena in attainable regimes, although they are outside the astrophysical scenario, can nevertheless validate the codes and guide our physical intuition for understanding the astrophysical world.

The development of specific experiments has been recognized as a key element in code validation [22]. Laboratory experiments can be constructed in such a way to reproduce the regimes attainable by numerical simulations. In particular several experiments have been set up and are under way that try to reproduce analogs of disks and jets [23-26]. Hopefully in the next future they will provide the necessary results to complete the code validation effort. At the same time the constant progress in high-performance computing and the use of grid networks will allow to extend the analysis of the parameter space toward the regimes of astrophysical interest.

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