

Position paper: Discontinuous Galerkin methods for exascale computing

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Discontinuous Galerkin (DG) methods have been extensively developed, analyzed and applied for convection-dominated partial differential equation (PDE) models in various applications including computational fluid dynamics, computational electro-magnetism, computational electronics, computational biology, etc. We refer to, e.g. [4, 6, 12] for more details. The simplest DG method for solving the transport equation

$$u_t + f(u)_x = 0$$

over the domain $[0, 1]$, discretized by a possibly non-uniform meshing $I_j = (x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}})$, with $0 = x_{\frac{1}{2}} < x_{\frac{3}{2}} < \dots < x_{N+\frac{1}{2}} = 1$, reads: find $u_h \in V_h = \{v : v|_{I_j} \in P^k(I_j)\}$ such that, for all $v_h \in V_h$,

$$\int_{I_j} (u_h)_t v_h dx - \int_{I_j} f(u_h)(v_h)_x dx + \hat{f}_{j+\frac{1}{2}}(v_h)_{j+\frac{1}{2}}^- - \hat{f}_{j-\frac{1}{2}}(v_h)_{j-\frac{1}{2}}^+ = 0.$$

Here the numerical flux $\hat{f}_{j+\frac{1}{2}} = \hat{f}((u_h)_{j+\frac{1}{2}}^-, (u_h)_{j+\frac{1}{2}}^+)$ is a suitably defined function of both the left limit and the right limit of the numerical solution u_h at the cell interface $x_{j+\frac{1}{2}}$, which is a possibly discontinuity point for functions in the finite element space V_h . The success of DG methods for various PDEs largely depends on suitable choice of the numerical flux functions and the resulting stability and accuracy properties of the DG methods thus derived. Time discretization can be achieved by explicit strong-stability-preserving (SSP) Runge-Kutta methods [5]. Exascale computing power is needed for simulations in high dimensions, e.g. for kinetic problems [3]. The DG methods have the following features (some of them are already explored in the literature, while others are still to be fully investigated), which make them ideal for exascale computing environments:

(1) DG methods are extremely local and compact. When an explicit time stepping is adopted, evolution of the polynomial in cell I_j depends only on the polynomials in I_j itself and in its immediate neighbors (I_{j-1} and I_{j+1} in the one-dimensional case) through the numerical fluxes $\hat{f}_{j-\frac{1}{2}}$ and $\hat{f}_{j+\frac{1}{2}}$, regardless of the order of accuracy or the polynomial degree k . The ratio of communications to local computations is extremely small. This makes DG method highly efficient in massively parallel environments and in GPUs [1, 11, 9]. This advantage is more prominent for higher order accurate DG methods, for example in the spirit of spectral finite element methods. When implicit time stepping must be used because of the need to relax the time step restriction, efficient preconditioning plus suitable iterative solvers again retain the advantage of DG in terms of small ratio of the cost of communications to the cost of local computations.

(2) DG methods are extremely friendly to h - p adaptivity. Arbitrary triangulations with hanging nodes are allowed for h -adaptivity, and polynomial degrees can be chosen differently and independently in different cells for p -adaptivity (e.g. [11]). Nonlinear stability proofs (for example the energy stability for scalar hyperbolic equations [8] and symmetric hyperbolic

systems [7]) hold for such general h - p adaptive cases. Error estimates for smooth solutions can also be obtained in such general cases.

(3) DG methods are friendly to multiscale problems or problems with solutions of special shapes, such as boundary or internal layers. Local non-polynomial or multiscale spaces (such as oscillatory functions or exponential functions) rather than polynomial spaces can be chosen for different cells at will. For example, exponential and trigonometric bases are used in [18] to solve problems with boundary or internal layers and problems with oscillatory solutions. Special basis based on WKB analysis is used in [15] to solve Schrödinger equation in a resonant tunneling diode, and special basis based on solutions of suitable cell problems is used in [13] to solve a class of second order elliptic problems with rough coefficients. Again, most stability results and error estimates hold for such general cases. For traditional continuous finite element methods, it is in general very difficult to enforce continuity of functions in the finite element space containing special basis functions across element interfaces in multi-dimensions. For discontinuous Galerkin methods this difficulty does not exist.

(4) DG methods are friendly to multi-physics environments. Different PDE models, or even non-PDE models such as molecular dynamics models, can be used in different domains, and they can be “glued together” through numerical fluxes in a DG setting. For example, kinetic models and macroscale moment models in different domains are glued together by discontinuous Galerkin methods, for both gas dynamics equations and semiconductor device simulation models in [2]. Nonlinear elastodynamics as the continuum description and molecular dynamics as another component at the atomic scale in different domains are glued together by discontinuous Galerkin methods for the multiscale modeling of dynamics of crystalline solids in [14].

(5) DG methods have redundant information (for example, at cell interfaces, left and right limits of the numerical solution both approximate the exact solution at this location; also, for central DG methods [10] there are two polynomials from which we can read values at any spatial location). This may turn out to be a crucial advantage for error tolerance in an exascale computing environment in which a small percentage of randomly distributed processors are expected to malfunction at any given time. We can use one piece of the redundant information instead of another piece which comes from the malfunctioned processor. A careful mathematical study on stability and accuracy of such modifications of the DG algorithm, perhaps in the probability sense, needs to be performed.

(6) Recent developments of DG methods, such as bound-preserving limiters which maintain accuracy and conservation [19, 20], and treatment of δ -singularities [16, 17], provide more evidence for the suitability of DG methods in exascale environments for complex physical and engineering applications. The bound-preserving limiters designed in [19, 20] can maintain conservation and accuracy, and can mathematically guarantee bound-preserving property of the numerical solution (e.g. positivity of density and pressure for Euler equations of gas dynamics). These bound-preserving limiters are especially useful to simulate solutions with δ -singularities, for other conventional limiters such as minmod type slope limiters severely smear δ -singularities. One advantage of these bound-preserving limiters is that they are completely local, namely their implementation is achieved element-wise. Therefore, addition of such limiters does not affect the efficiency of DG algorithms in exascale environments.

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