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14. ABSTRACT
A thoroughly validated, robust, and efficiently solver for the electromagnetics problem continues to be extended to provide a basic field solver for the EM-PIC problem. This has resulted in a first generation of a DG-FEM based PIC method on unstructured grids. The particle mover relies on high-order interpolation, efficient local search algorithms to locate the particles, and a level set approach to implement elastic/inelastic interactions with boundaries. Charge and current, redistribution computations use large smooth weight functions, dramatically decreasing the number of particles needed in a computational cell as compared to the compared to the simple redistribution schemes typically used. A large smooth Gaussian-like distribution function is used as a regularized for the particle per particle to sums the influence of the particles into the charge and current density field variables. Currently, a constant particle influence-radius ensures charge conservation in the domain, but requires a variable number of element.

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High-Order Accurate Particle-in-Cell (PIC) Methods on Unstructured Grids with Applications to Microwave Generation and Accelerator Modeling.

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October 1, 2005 - May 31, 2006

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1 Background

The reliable, accurate, and efficient computational modeling of plasma dynamics remains a challenge of very significant proportions but also with a broad range of possible applications, e.g., high-power microwave generation; large scale particle accelerators; fusion energy, both by means of magnetic confinement and laser ignited devices; and a variety of plasma based technology as well as numerous problems of mainly military interest. This warrants that significant resources be spend on the continued development of accurate, robust, and efficient tools for the modeling of this broad range of phenomena and scales.

The direct and straightforward solution of many of the problems, at least in the collisionless region, could in principle be accomplished by solving the phase-space Vlasov equation

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla_x f + \boldsymbol{F} \cdot \nabla_v f = 0 \ , \tag{1}$$

where $f(\boldsymbol{x}, \boldsymbol{v}, t)$ is the probability density, one for each charged particle species, and the force, $\boldsymbol{F}$, is the electromagnetic Lorenz force

$$\boldsymbol{F} = \frac{q}{m}\left[\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B}\right] \ ,$$

for each particle type of charge q and mass m. In case of relativistic speeds, the mass needs to be corrected according to special relativity. The electromagnetic fields, $(\boldsymbol{E}, \boldsymbol{B})$ satisfy Maxwell equations

$$df dx\boldsymbol{E}t = \nabla_x \times \boldsymbol{B} + \boldsymbol{J} \ , \ \frac{\partial \boldsymbol{B}}{\partial t} = -\nabla_x \times \boldsymbol{E} \ , \tag{2}$$

where we have assumed vacuum conditions at unity for simplicity, i.e., $\varepsilon_0 = 1, \mu_0 = 1$, and the speed of light is normalized to one. The fields are further constrained through

$$\nabla_x \cdot \boldsymbol{E} = \rho \ , \ \nabla_x \cdot \boldsymbol{B} = 0 \ , \tag{3}$$

where the former ensures charge conservation through

$$\frac{\partial \rho}{\partial t} + \nabla_x \cdot \boldsymbol{J} = 0 \ ,$$

for the space charge $\rho(\boldsymbol{x}, t)$ and current density $\boldsymbol{J}(\boldsymbol{x}, t)$.

This system needs to be solved in the fully dynamic range for cases where the particles are close to relativistic speeds as is the case for many areas of modern technology, e.g., high-power microwave generation, accelerator modeling and fusion applications.

However, the 6+1 dimensional nature of Eq.(1) and the very complex phase space dynamics, essentially implies that direct modeling remains out of reach for problems in complex geometries and of realistic complexity. On the other hand, this approach offers a direct measure stick against which to compare new methods and evaluate their performance.

The practical difficulties associated with the direct solution of the above system has encouraged the development of a number of indirect approaches to solve this type of problems. The most widely used approach is the particle-in-cell method (PIC) which is based on a sampling technique. Here, one samples, using a large number of particles, the local distribution function, $f(\boldsymbol{x}, \boldsymbol{v}, t)$, in velocity space and then move these particles around in a fully Lagrangian fashion using Newton's law of motion. In other words, one represents the first two moments, $\rho(\boldsymbol{x}, t)$, and $\boldsymbol{J}(\boldsymbol{x}, t)$, as

$$\rho(x,t) = \sum_k \tilde{\rho}_k(x,t) \ , \ \ J(x,t) = \sum_k \tilde{J}_k(x,t) \ ,$$

where $\tilde{\rho}_k$ and $\tilde{J}_k$ represent the charge and and current originating from particle k. Each of these k particles are them moved according to

$$\frac{d^2 m_k x_k}{dt^2} = \rho_k \left[E(x_k) + v_k \times B(x_k) \right] \ .$$

Thus, the computational work is shifted from a 6+1 dimensional problem to a 3+1 problem but with a large number of particles moving freely around and for which there is constant interaction between the fields and the particles. The simple sampling approach taken in this technique also means that a very large number of particles has to be used to limit the classic $1/K$ sampling noise.

While these methods generally are efficient and has served the community well, they typically rely on the use of relatively simple grids and low order accurate methods, in particular for the fully electromagnetic problem, for the field solvers – typically 2nd order finite difference or finite element methods, the latter mainly for the low-speed case. As a consequence of this, many of these algorithms are now being stretched due to the quest to resolve problems with a large range of active scales, both in time and space. Further complications arise when the interaction between geometries and the fields become important such as in magnetrons and klystons for microwave generation, as well as problems associated with inherent numerical properties of the low order schemes, e.g, numerical dispersion and numerical Cherenkov radiation.

In this proposal we have consider the continued development and maturation of a computational kernel based on the discontinuous Galerkin method (DG-FEM) for the field solver while various alternatives are possible for the particle models. This approach has several advantages for applications of the type discussed in this effort, i.e., their ability to easily handle complicated, electrically large geometries and complex boundary conditions, their flexibility to support nonconforming *hp* adaptivity, and the ability to efficiently deal with both the high-speed fully electromagnetic problem and the low speed problem within one formulation.

DG-FEM have experienced an explosion in interest over the last decade, although with relatively limited impact in plasma physics applications. This is in particular the situation for particle-mesh methods where, as discussed above, classic 2nd order accurate PIC methods remain the dominating tool in spite of well known inherent problems.

As we shall discuss shortly, we have made significant progress towards the development of an alternative to the current simulation tools. Ultimately, the hope is that the continuation of this effort will result in a software tool of sufficient robustness and versatility to be useful to AFRL researchers in the development and evaluation of new technology, critical to the mission of USAF.

2 Main Developments

A thoroughly validated, robust, and efficiently solver for the electromagnetics problem continues to be extended to provide a basic field solver for the EM-PIC problem. This has resulted in a first generation of a DG-FEM based PIC method on unstructured grids. The particle mover relies on high-order interpolation, efficient local search algorithms to locate the particles, and a level set approach to implement elastic/inelastic interactions with boundaries. Charge and current redistribution computations use large smooth weight functions, dramatically decreasing the number of particles needed in a computational cell as compared to the simple redistribution schemes typically used. A large smooth Gaussian-like distribution function is used as a regularized for the particle per particle to sums the influence of the particles into the charge and current density field variables. Currently, a constant particle influence-radius ensures charge conservation in the domain, but requires a variable number of elements per particle for weighing purposes depending on the size of the elements. The element's that are being influenced by a particle are determined in a pre-processing stage by finding the elements connected to the node nearest to the particle.

In this effort, we have primarily concerned ourselves with three topics

- *Time-advancement.* We have, with great success, implemented a implicit-explicit Runge-Kutta methods [?] in which the full EM part, Eq.(2), is done implicitly, while the charge dynamics and current deposition is done explicitly. This removes all grid induced stiffness and enables one to effectively model geometrically complex problems. However, stiffness introduced by physical properties, i.e., high electron cyclotron frequencies or small Debye shielding lengths still imposes certain constraints on the time step. This has lead to significant speedups for classes of problems where hyperbolic divergence cleaning is the preferred approach. Furthermore, this approach is well suited for problems in complex geometries.

  To completely overcome stiffness, including that introduced by physical phenomena, we have also considered a full implicit moment method. This is highly efficient for problems in strong magnetic fields and for problems with particles of different charge and mass, e.g., electron-ion mixtures. Currently, this method is at best 2n dorder accurate and we are working to address this

  Both methods have been carefully validated and their design accuracy confirmed for simple test problems, as exemplified in Fig 1.

- *Techniques for phase-spase control* A key concern in methods of this type is the very high number of particles typically used. This normally controls the computational cost entirely. We have pursue a solution to this by investigating alternative ways of representing particles, techniques for splitting and combining particles and, finally, ways of estimating the phase-space error.

  The most fruitful approach appears to be that of solving a problem twice in different ways and then comparing they two. For this, one needs an alternative equation and we propose to consider the δf-equation

$$\frac{\partial \delta f}{\partial t} + \boldsymbol{v} \cdot \nabla_x \delta f + \boldsymbol{F} \cdot \nabla_v \delta f = -\boldsymbol{v} \cdot \nabla_x f_0 + \boldsymbol{F} \cdot \nabla_v f_0 \ ,$$

  i.e., it is the Vlasov equation (locally) linearized around some f_0. Clearly, if f_0 is kept fixed in time, this will be expensive to solve. However, if we use non-parametric estimation to re-evaluate f_0 at fixed temporal intervals, one can solve the above linearized Vlasov equation with a low number of particles. The predicted changes in δf will provide a measure of the phase-space dynamics/sensitivity and we can then compare this with the current local sampling of phase-space to recover a measure of whether phase-space is adequately sampled.

  An attractive alternative to this is to explore appropriate fluid models for the systems being modeled and exploit the fact that DG-FEM is ideally suited for solving such fluid models, often given as conservation laws. Furthermore, since the cost of solving the fluid model is much less that the kinetic model, we propose to run both models simultaneously. The output

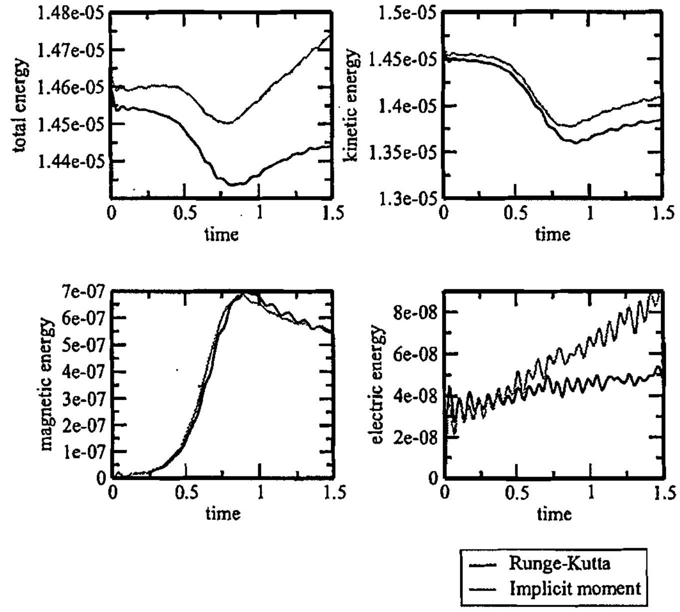

Figure 1: Direct comparison of a DG-FEM based scheme with two different implicit temporal integration schemes.

from the fluid model then provides information about the first few moments of the kinetic simulation and a comparison between the results from the fluid model and the kinetic model can be used to identity regions close to equilibrium, hence requiring just a few particles, and strongly kinetic regions where more particles are needed. Since the fluid solver is used for error estimation only, it can be solved with marginal resolution and restarted with initial conditions from the kinetic solver at given interval. This will also provide a suitable return place in case the estimator determines that the physics is severely under resolved.

Both of these techniques are currently being explored further in a carefully designed experiment to judge which of the two is advantageous.

- *Thorough validation* The scheme has been implemented and extensively tested in two spatial dimensions, both for low-speed and high-speed test cases and applications, including classic cases such as plasma waves, Landau damping, two-stream instabilities, relativistic Weibel instabilities etc. In all these cases, careful comparisons have been done with standard methods based on finite difference methods, yields very good agreement. An example is shown in Fig. 2 where we show the direct comparison for the relativistic Weibel instability

  Following this extensive testing, we have demonstrated the flexibility and robustness of the scheme for two-dimensional simplification closer to problems of realistic complexity. An example of this is shown in Fig.3 where we show the modeling of a relativistic magnetron.

  Many other benchmarks have been considered, including bore-magnetrons and non-dissipative magnetic recognection.

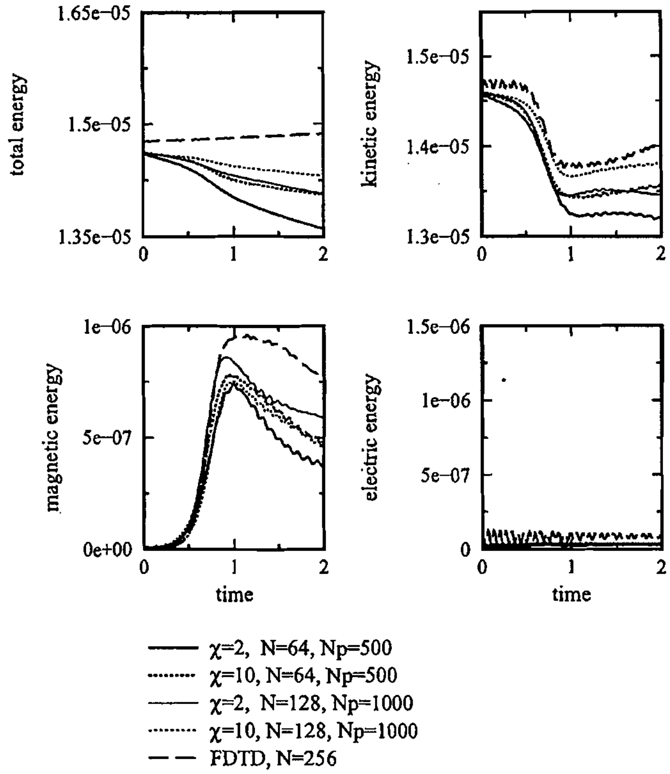

Figure 2: Direct comparison of a DG-FEM based scheme with a classic finite difference based scheme for modeling of the Weibel instability.

3 People Supported by Award

- Professor Jan S Hesthaven, PI
- Dr Gustav Jacobs, Postdoctoral researcher, now assistant professor at San Diego State University
- Akil Narayan. Graduate student.

4 Talks and Publications

- *Talks* AIAA, Reno, 2006. SIAM Annual Meeting, Boston, 2006. Technical University of Denmark, 2005. University of Strasbourg, France, 2006. 13 talks by Dr G. Jacobs as part of his interview rounds for a faculty position.
- *Publications*

  G. Jacobs and J.S. Hesthaven, 2005, *High-Order Nodal Discontinuous Galerkin Particle-in-Cell Methods on Unstructured Grids*, J. Comput. Phys. **214**(2006), 96-121.

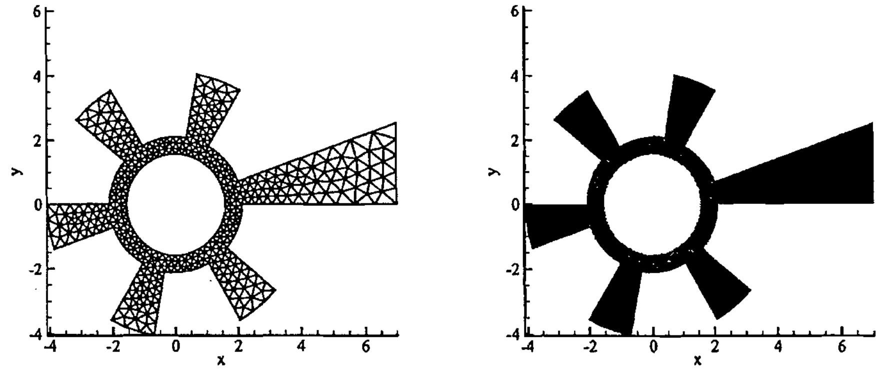

Figure 3: Left) Grid for 2D version of A6 relativistic magnetron. Right) Charge density in the magnetron, running in the 2π mode. Both results computed using a DG-FEM for full PIC

G. Jacobs, G. Lapenta, and J.S. Hesthaven, 2006, *High-Order Nodal Discontinuous Galerkin Particle-in-Cell Methods for Modeling of Weibel Instabilities*, AIAA paper, Reno, 2006.

Two more papers are currently being finished, devoted to the development and validation of the time-stepping schemes, and a detailed validation study of geomagnetic reconnection benchmark (GEM).