Final Report for Center for Tokamak Transient Simulations at USU

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Contents

1 Introduction

Providing plasma fluid codes like NIMROD[1] with continuum drift kinetic (CDK) physics[2] that is quantitatively valid and computationally feasible throughout the spatial domain is difficult. Work at Utah State University (USU), in collaboration with the Center for Tokamak Transient Simulations (CTTS), focused on applying CDK closures in disruption-related calculations. Three examples where kinetic physics is paramount are (1) the electron stress tensor closure in Ohms law for accurately describing neoclassical tearing mode (NTM) evolution, (2) runaway electron (RE) density (n_{RE}) and current ($\mathbf{j}_{RE}$) moments in NIMROD's extended MHD model for self-consistent evolution of RE populations during disruptions and, (3) energetic ion effects on a myriad of MHD instabilities. While NTM simulations and continuum and PIC approaches to energetic ions in NIMROD have been a major goals of USU's closure work for several years, the development of self-consistent CDK RE capability[3] in NIMROD was started and extended considerably during the CTTS effort. Some goals of CDK RE in NIMROD are to explore the effects of the 2D relativistic phase space in 4D simulations and compare with NIMROD's fluid RE model[4].

Four publications and two PhD theses came out of the USU CTTS effort. There are several student authors and co-authors in the publications, namely, Tyler Markham (PhD), Trevor Taylor (PhD), and Brett Adair, all graduate students at USU and Joseph Jepson, who did his undergraduate research using NIMROD with Dr. Held at USU before moving on to the University of Wisconsin to work with Dr. Chris Hegna (in collaboration with Dr. Held). The USU computational/theoretical fusion group takes its job of training the next generation of plasma fusion physicists for the MFE community very seriously. We include a comprehensive list of relevant work here and summarize the contents in the remainder of this report.

1. J.-Y. Ji, J. A. Spencer, and E. D. Held, "Exact irreducible moments of the Landau collision operator in the random-velocity moment expansion", *Plasma Res. Express*, **2**, 015013 (2020).

2. J. A. Spencer, B. Adair, E. D. Held, J-Y Ji and J. R. Jepson, "Accurate numerical, integral methods for computing drift-kinetic Trubnikov-Rosenbluth potentials", *J. Comput. Phys.*, **450**, 110862 (2022).

3. J. R. Jepson, C. C. Hegna, E. D. Held, J. A. Spencer and B. C. Lyons, "Benchmarking NIMROD continuum kinetic formulations through the steady-state poloidal flow", *Phys. Plasmas*, **28**, 082503 (2021).

4. Joseph R. Jepson, Chris C. Hegna, Eric D. Held, Carl R. Sovinec, J. Andrew Spencer, Eric C. Howell, "An analysis and successful benchmarking of the Chapman-Enskog-like (CEL) continuum kinetic closure approach algorithm in NIMROD", *submitted to Computer Physics Communications in January 2024.*

5. Relativistic, Continuum Drift-Kinetic Capability in the NIMROD Plasma Fluid Code[3], PhD thesis defended in December 2022 (Available at `https://digitalcommons.usu.edu/etd/8683/`).

6. Serendipity Shape Function for Hybrid Fluid/Kinetic-PIC Simulation[5], PhD thesis defended in October 2022 (Available at `https://digitalcommons.usu.edu/etd/8652/`).

2 Analytic form for Coulomb collision operator for arbitrary flow ordering

We begin our USU CTTS summary with some nice theory work that was led by Dr. Jeong-Young Ji and funded by a supplemental SciDAC proposal to USU. The goal was to develop accurate closure relations to capture runaway electron effects. For an arbitrary relative flow velocity between electrons and ions $V_{ei} = V_e - V_i$, we developed a formalism to calculate the collisional moments of the Landau (Fokker-Planck) operator by deriving explicit formulas for the analytic collision coefficients expressed in terms of finite series in V_{ei}. Since the moment expansion is performed in each fluid frame with a shifted Maxwellian distribution function, the formulas are exact for arbitrary V_{ei}. The formulas involve only algebraic expressions and can be implemented in symbolic computation programs such as Mathematica and Maple. The work[6] was published in

J.Y. Ji, J. A. Spencer, and E. D. Held, "Exact irreducible moments of the Landau collision operator in the random velocity moment," Plasma Research Express, 2 (2020).

The results may be used in situations where the electron distribution has developed a significant flow moment, on the order of the electron thermal speed, but a relativistic treatment is not yet necessary. Corrections terms in V_{ei} are critical for handling the early-in-time development of a runaway electron (RE) distribution that often accompanies disruptions.

The exact calculation of the collisional moments significantly modifies the Braginskii closure relations at a finite value of $\mathbf{V}_{\rm ei}$. Figure 1 shows that the friction coefficient of Braginskii's[7] closures is valid only when $V_{\rm ei}$ is much smaller than the electron thermal speed $v_{T\rm e}$. Note that the friction force is proportional to $V_{\rm ei}$ for $V_{\rm ei} \lesssim 0.2 v_{Te}$ in Fig. 1 and the collision coefficients are constant only when $V_{\rm ei} \ll v_{Te}$ in Figures 1, 2 and 3. For $V_{\rm ei} \sim v_{T\rm e}$, the exact collision coefficients are significantly different from the linear coefficients.

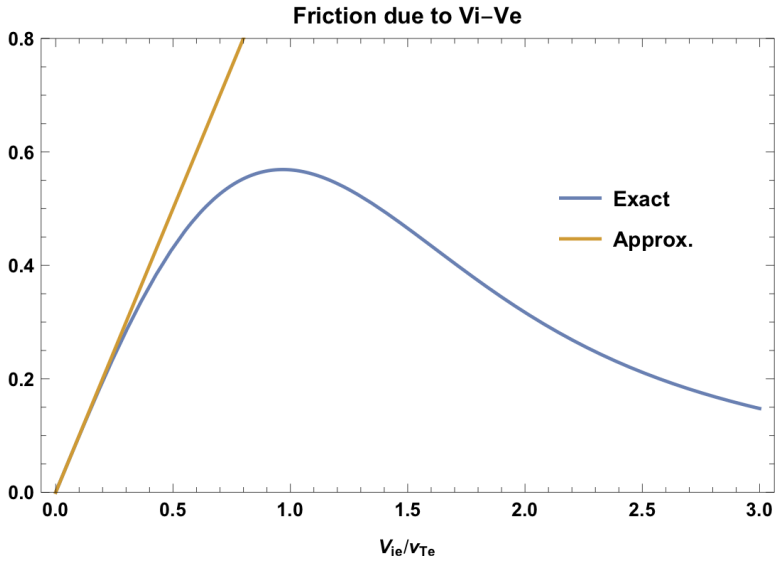

Figure 1: Friction force due to the relative flow velocity shows significant modifications to Braginskii theory as a function of $V_{\rm ei} \sim v_{T\rm e}$.

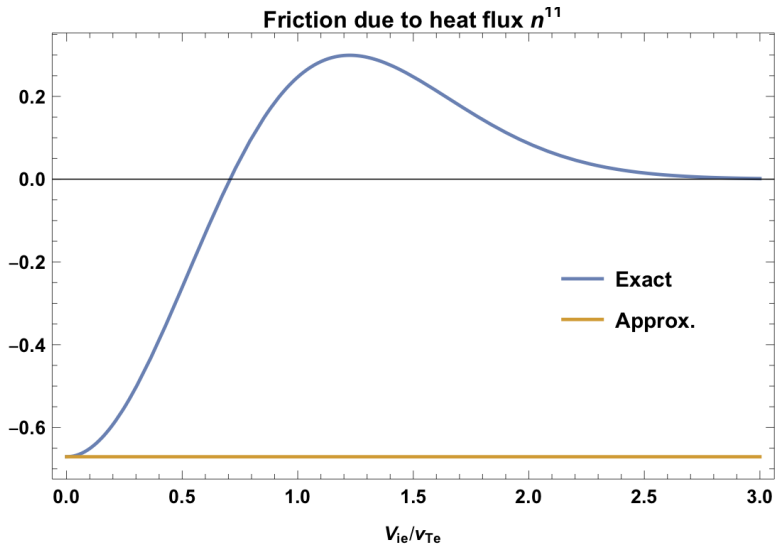

Figure 2: Friction coefficient of the heat flux shows significant modifications to Braginskii theory as a function of $V_{\rm ei} \sim v_{T\rm e}$.

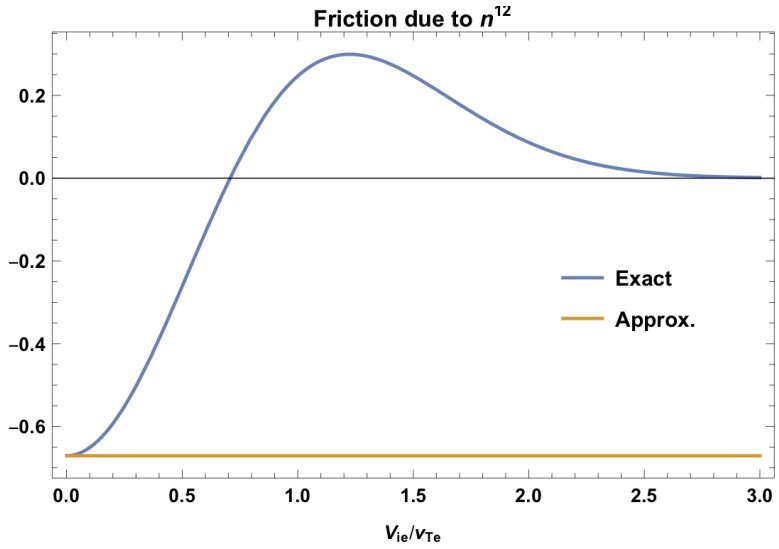

Figure 3: Friction coefficient of the heat-weighted heat flux shows significant modifications to Braginskii theory as a function of $V_{\rm ei} \sim v_{T\rm e}$.

3 Improved Rosenbluth potential algorithm for NIMROD CDK

While working on a comprehensive, hybrid fluid/kinetic capability for simulating NTMs in NIMROD, we discovered that improvements were needed in NIMROD's CDK implementation of the Rosenbluth potentials for the field portion of the collision operator. Drs. Spencer and Held put a great deal of effort into constructing a more efficient and accurate approach to computing the Rosenbluth potentials. Part of this work entailed finding a robust method for integrating over singularities in the Green's functions of the velocity space Poisson equation. We implemented a numerical splitting technique, which was adapted from the astrophysics community[8] to compute gravitational potentials from axisymmetric sources. We also derived a series expansion that reduced the dimensionality of a large portion of the calculation. The results of our algorithm were compared to those of a third party general adaptive integrator to demonstrate convergence to a desired accuracy. Our algorithm was significantly more efficient, and able to quickly evaluate results for cases where the third party software was not able to complete the calculation due to running out of computer memory. This effort resulted in the JCP publication[9]

J. A. Spencer, B. Adair, E. D. Held, J-Y Ji and J. R. Jepson, "Accurate numerical, integral methods for computing drift-kinetic Trubnikov-Rosenbluth potentials", *J. Comput. Phys.*, **450**, 110862 (2022).

During this research, we found a simplification of the series expansion that allowed us to reduced the dimensionality of the evaluation of the Rosenbluth potentials. It hinged on how efficiently Legendre polynomials resolve localized structures of the velocity distribution function in pitch angle. As it turned out, a Rosenbluth potential implementation with an extensive Legendre expansion was able to handle trapped/passing boundary (*tpb*), finite-element (FE) grids in pitch angle. These *tpb* grids provide excellent resolution of the RE distribution at the trapped/passing boundary and are critical for an accurate account of neoclassical transport including the bootstrap current, J_{BS}. Figure 4 shows the electron distribution function (left), F_e, from a bootstrap current calculation for a lower-collisionality, DIII-D-like equilibrium. Sharp variations in F_e near the *tpb* (black) are well-resolved by an FE grid (red) with one cell in negative-passing, trapped and positive-passing space and natural packing of Gauss-Lobatto-Legendre (GLL) nodes at the *tpb*. The right plot indicates the improved convergence of *tpb* grids as degrees of freedom (dof) are added in ξ. Importantly, *tpb* grids with 80 dofs are already more accurate than 380 dofs associated with a uniform GLL grid or Legendre polynomials.

We note that significant contributions to this effort were provided by Brett Adair, who was funded by CTTS money at USU. Also, careful testing of the implementation was carried out by Joseph Jepson, who was advised by Dr. Chris Hegna at UW-Madison. The 5 years plus collaboration between Held (USU), and Jepson and Hegna at UW has proven profitable for continuum CDK development in NIMROD.

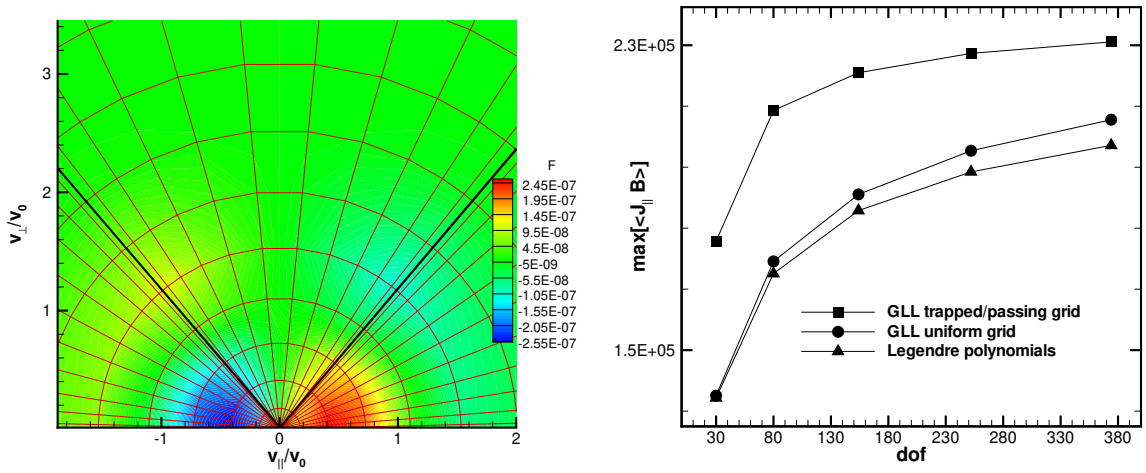

Figure 4: Left plot shows the well-resolved variation in F_e at the trapped/passing boundary (black lines) with *tpb FE grids*. The maxima in the J_{BS} profiles (right) indicate the substantially improved convergence afforded by *tpb* grids as degrees of freedom (dof) are added in ξ.

4 Improved time-stepping algorithm for coupled NIMROD-fluid/CDK system

One CDK method that has been implemented in the plasma fluid code NIMROD is the Chapman-Enskog-like (CEL) approach[10, 11, 12]. This is a continuum kinetic approach that partitions the velocity distribution function, $f(\mathbf{x},\mathbf{v},t) = f_{NM}(\mathbf{x},\mathbf{v},t) + f_{\mathrm{M}}(\mathbf{x},\mathbf{v},t)$ into a Maxwellian part, f_{M}, parameterized by the density, n, macroscopic flow velocity, $\mathbf{V}$, and temperature, T, and a distinct kinetic distortion, f_{NM}. The fluid quantities evolve according to the NIMROD's fluid implementation and the closures are provided by moments of f_{NM}, which evolves according to the CEL kinetic equation. That is to say, the kinetic distortion is governed by a form of the kinetic equation in which the Maxwellian moments have been removed. This ensures that during the evolution of the distribution function, f_{NM} is always orthogonal to f_{M}. While this happens exactly in terms of analytics, we have found that numerical "cleaning" of the Maxwellian moments of f_{NM} is necessary during tightly-coupled, hybrid fluid/CEL kinetic simulations[12].

Since the details of a fully self-consistent hybrid fluid/CEL-DKE implementation are quite technical, we begin by discussing the intricacies of a simpler problem, namely, the coupling between T and f_{NM}. In this model, we evolve the electron and ion temperatures in the presence of a static magnetic island in slab geometry. The temperature equation for this model is

$$\frac{3}{2}n\frac{\partial T}{\partial t} = \kappa_{\perp}\nabla\cdot\left[\left(\mathbf{I}-\mathbf{bb}\right)\cdot\nabla T\right] - \nabla\cdot\mathbf{q}_{\parallel} \tag{1}$$

where $\kappa_{\perp}$ is a perpendicular thermal conductivity and the parallel heat flux is given by $\mathbf{q}_{\parallel} = \frac{m}{2}\int d\mathbf{v} v^2 v_{\parallel} f_{NM}$. The kinetic distortion is governed by the CEL drift-kinetic equation

$$\begin{aligned}\frac{\partial f_{NM}}{\partial t} + \mathbf{v}\cdot\nabla f_{NM} - \frac{1-\xi^2}{2\xi}\mathbf{v}_{\parallel}\cdot\nabla\ln B\frac{\partial f_{NM}}{\partial \xi} - \frac{s}{2}\left(\mathbf{v}_{\parallel}\cdot\nabla + \frac{\partial}{\partial t}\right)\ln T\frac{\partial f_{NM}}{\partial s} \quad &= \\ C + \left(\frac{5}{2} - s^2\right)\mathbf{v}_{\parallel}\cdot\nabla\ln T f_{\mathrm{M}} + \frac{2}{3nT}\left(s^2-\frac{3}{2}\right)\left(\nabla\cdot\mathbf{q}_{\parallel}\right) f_{\mathrm{M}}.\end{aligned} \tag{2}$$

Here we introduce normalized speed and pitch-angle coordinates, $s = |\mathbf{v}|/v_T$ $\xi = \mathbf{v}\cdot\mathbf{B}/|\mathbf{v}||\mathbf{B}|$

The first three terms on the left side of Eq. 3 are the time derivative, free streaming and bounce terms, respectively. The last term on the left side is needed to scale the velocity domain as the temperature changes due to the speed coordinate being normalized by the thermal speed. On the right side, we have the collision operator, and Maxwellian drives that are formed as the result of projecting out the temperature moment from the kinetic equation. For comparison, Braginskii's closure for the parallel heat flux is $\mathbf{q}_{\parallel} = -\kappa_{\parallel}\left(\mathbf{b}\cdot\nabla T\right)\mathbf{b}$ where $\kappa_{\parallel}$ is Braginskii's parallel thermal conductivity.

The time scale of NTM dynamics proceeding a disruption can be on the order of hundreds of milliseconds, whereas the electron transit time is sub-microsecond. Therefore, we sought an implicit time discretization scheme that allows large time steps to be taken. However, Eq. 3 possesses a strong nonlinear coupling of T and f_{NM}. This enters through the collision operator, the parallel temperature gradient drive term, and in fact, in most terms in Eq. 3 due to the thermal speed normalization of the velocity space. A nonlinear coupling also comes from Eq. 1 through the heat flux, again from the velocity normalization. Therefore, a lot of work needed to be done to advance the temperature and kinetic distortion implicitly and simultaneously.

In NIMROD's implementation, the CEL kinetic equation is solved at a set of collocation points in speed, $F_i(\mathbf{x},\xi,t) = F(\mathbf{x},s_i,\xi,t)$. These points correspond to a set of quadrature nodes used to compute moments of the kinetic distortion, which closes the fluid equations. Both spectral and finite element

(FE) methods have been implemented to solve for the pitch-angle dependence of F[**?**]. The spectral method uses Legendre polynomials, which are eigenfunctions of the linearized Coulomb collision operator, hence a common choice in drift kinetic codes. The FEM uses Lagrange or Gauss-Legendre-Lobatto (GLL) polynomials with uniform grid spacing, or FE vertex nodes located at the local trapped/passing boundary. As shown earlier, these *tpb* grids offer superior resolution in neoclassical transport calculations, much better than the spectral Legendre approach, which had been applied for decades in drift kinetic codes.

In either case, we can expand the kinetic distortion in terms of the pitch-angle basis functions, $P_j(\xi), F_i(\mathbf{x},\xi,t) = \sum_{j=0}^{\mathrm{dof}} F_{i,j}(\mathbf{x},t) P_j(\xi)$ where dof is the number of degrees of freedom in pitch-angle. The kinetic distortion's spatial dependent coefficients and temperature are expanded in terms of NIMROD's usual finite elements and Fourier modes,

$$F_{i,j}(R,Z,\phi,t) = \sum_{k=0}^{N} \left\{ F_{i,j,k,l=0}(t) + 2\Re e \left[\sum_{l>0} F_{i,j,k,l}(t)\, \mathrm{e}^{il\phi} \right] \right\} \alpha_k(R,Z) \tag{3}$$

and

$$T(R,Z,\phi,t) = \sum_{k=1}^{N} \left\{ T_{k,l=0}(t) + 2\Re e \left[\sum_{l>0} T_{k,l}(t)\, \mathrm{e}^{il\phi} \right] \right\} \alpha_k(R,Z) \tag{4}$$

where ϕ is the toroidal angle and $\alpha_k(R,Z)$ are N finite element basis functions over the poloidal plane.

Since the number of degrees of freedom in pitch-angle is almost always chosen to be greater than the number of fluid quantities evolved in NIMROD, we combine fluid quantities with the kinetic distortion conveniently by extending the kinetic distortion solution array by one virtual speed point, s_0, and allowing the fluid quantities to occupy some of the corresponding pitch-angle degrees of freedom. For example, electron temperature sits in the first degree of freedom of the virtual speed point, $T(R,Z,\phi,t) = F_{0,0}(R,Z,\phi,t)$ and T_i sits in the second for the coupled T/f_{NM} system.

We have implemented a distributed memory parallelism over speed collocation points which is analogous to NIMROD's Fourier mode parallelism. Subsets of processors solve the CEL=DKE at single (or multiple) speed points and then communicate results for taking moments. Combining the temperature with the kinetic distortion by adding a virtual collocation point has been met with the challenge of effectively preconditioning the linear system complicated by the fact the temperature now couples to the rest of the distribution function through the heat flux, the Maxwellian drives, and the couplings due to our speed normalization. Effective preconditioning is a matter of ongoing research (mainly to use GPU acceleration to improve computation times for preconditioning).

In order to solve the highly nonlinear system of equations (Eq. 1 and Eq. 3), we implemented Newton's method. For time discretization, we use a theta-centered, semi-implicit finite difference scheme. This involves the solution of nonlinear algebraic equations. If we use a superscript, n, to denote the time step, t_n, then the solution vector for which NIMROD solves is the set of unknown coefficients, $F^{n+1}_{i,j,k,l} \equiv F_{i,j,k,l}(t_{n+1})$, where the i=0 and j=0 coefficients correspond to the coefficients in the temperature expansion. Using vector notation to represent the solution vector, $\mathbf{f_{NM}}^{n+1}$, whose components are $F^{n+1}_{i,j,k,l}$, and discretizing using the FE /Fourier/collocation method, we arrive at a set of nonlinear algebraic equations that can be written in the form $\mathbf{A}\left(\mathbf{F}^{n+1},\mathbf{F}^{n}\right) = \mathbf{b}\left(\mathbf{F}^{n}\right)$ where $\mathbf{A}$ and $\mathbf{b}$ are nonlinear operators. Newton's method is an iterative method. We label iterates with a second superscript, $\mathbf{F}^{n+1,m}$, and the converged solution as $\mathbf{F}^{n+1,\infty}$. Newton's method applied to our set of nonlinear, partial differential equations solves the following system of linear equations,

$$\left.\frac{\partial \mathbf{A}(\mathbf{F},\mathbf{F}^{n,\infty})}{\partial \mathbf{F}}\right|_{\mathbf{F}=\mathbf{F}^{n+1,m}} \cdot \left(\mathbf{F}^{n+1,m+1} - \mathbf{F}^{n+1,m}\right) = \mathbf{b}\left(\mathbf{F}^{n,\infty}\right) - \mathbf{A}\left(\mathbf{F}^{n+1,m},\mathbf{F}^{n,\infty}\right) \tag{5}$$

where $\partial \mathbf{A}\left(\mathbf{F}, \mathbf{F}^{n,\infty}\right) / \partial \mathbf{F}|_{\mathbf{F}=\mathbf{F}^{n+1,m}}$ is the Jacobian matrix of $\mathbf{A}$.

The left side of Eq. 5 is the linearized form of the nonlinear operator, $\mathbf{A}$. This linear system is solved using NIMROD's matrix-free, Generalized Minimum Residuals method normally. This means the full Jacobian matrix is never explicitly formed, nor its inverse. All that is needed is that action of the Jacobian matrix on the vector of unknowns. The iterative loop envelopes the calls to the linear solver. Within the iterative loop and outside the linear solver are calls to subroutines that update the right side of Eq. 5 and pre-computed quantities needed to form the action of the Jacobian matrix, such as the collision operator matrices that couple degrees of freedom in velocity space. A preconditioning matrix is computed at most once per time step, but can often be reused over multiple (as many as 50 in 4D nonlinear compuations) time steps.

Implementing the simultaneous advance of temperature and kinetic distortion required some unfamiliar linearization of the operator $\mathbf{A}$. For example, temperature derivatives must be taken of the kinetic equation. Kinetic distortion derivatives must also be taken of the heat flux in the temperature equation. Without these linearizations, Newton's method fails to converge because the resulting linear system is not a true linearization of the nonlinear system. As an example of the more complex linearizations, consider the temperature derivative of the collision operator. The temperature derivative of the test particle collision operator, $C\left[f_{NM}, f_{\mathrm{M}}\right]$, is done simply by taking a temperature derivative of the collision frequency, which is a coefficient of the collision operator. This was easily done analytically. However, the temperature derivative of the field operator, in particular, the collisions of the background electron Maxwellian off the ion kinetic distortion, $C\left[f_{\mathrm{e}}^{\mathrm{M}}, f_{NMi}\right]$, is much more involved due to temperature ratios that appear in evaluating the electron distribution function at speeds normalized by the ion thermal speed, $s_{\mathrm{e}} = v_{T\mathrm{i}} s_{\mathrm{i}} / v_{T\mathrm{e}}$. To avoid these complications and potential bugs that might be introduced in such an effort, the temperature derivative of the field operator is performed numerically rather than analytically. This was easy to implement and check. We verified the implementation by comparing numerical derivatives of the test particle operator with analytic derivatives. Unusual linearizations still remain for terms like the collisional friction, where we plan to adopt numerical derivatives for these terms as well.

4.1 Full coupling of CEL-DKEs and NIMROD's fluid model.

Work to implement a fully coupled, electron and ion CEL-DKE/NIMROD fluid system began in 2016. CTTS funding augmented this effort considerably with the hire of Dr. J. Andrew Spencer at USU in October of 2017. Dr. Spencer finished his PhD work with Dr. Held at USU in 2012. His work focused on a NIMROD-*esque* implementation of the Fokker-Planck equation. Dr. Spencer's NIMROD expertise has served the CTTS effort very well. Throughout the CTTS project, Drs. Held and Spencer have collaborated with Drs. Carl Sovinec and Chris Hegna at UW-Madison. This collaboration included important contributions from Dr. Hegna's student, Joseph Jepson, who began work on NIMROD CDK while an undergrad at USU. Development work by Held, Spencer and Jepson, supported at USU by CTTS funds, has led to a complete, self-consistent, and fully coupled implementation of electron and ion CEL closures in NIMROD. This is the first coupling of its kind in any plasma fluid code in the international MFE community.

In order to highlight the significance of this, we state the full CEL-DKE[10]

$$\frac{\partial f_{\rm NM}}{\partial t} + v_0 s\xi \mathbf{b}\cdot\nabla f_{\rm NM} - \frac{1-\xi^2}{2\xi} v_0 s\xi \mathbf{b}\cdot\nabla \ln B \frac{\partial f_{\rm NM}}{\partial \xi} \tag{6}$$
$$+\frac{v_0}{2}\left(\mathbf{b}\cdot\nabla \ln n\right)\left[\xi\frac{\partial f_{\rm NM}}{\partial s} + \frac{1-\xi^2}{s}\frac{\partial f_{\rm NM}}{\partial \xi}\right] - s\left[\xi\mathbf{b}\cdot\nabla + \frac{\partial}{\partial t}\right]\ln v_0 \frac{\partial f_{\rm NM}}{\partial s}$$
$$= \langle C\left(f\right)\rangle + [\left(\frac{5}{2} - s^2\right) v_0 s\xi \mathbf{b}\cdot\nabla \ln T + \frac{v_0 s\xi}{nT}\mathbf{b}\cdot\left[\frac{2}{3}\nabla\pi_{\parallel} - \pi_{\parallel}\nabla \ln B - \mathbf{R}\right]$$
$$+2s^2\left(\frac{3}{2}\xi^2 - \frac{1}{2}\right)\left[\frac{1}{3}\nabla\cdot\mathbf{u} - \mathbf{b}\mathbf{b}\cdot\nabla\mathbf{u}\right] + \frac{2}{3nT}\left(s^2 - \frac{3}{2}\right)\left[\mathbf{b}\cdot\nabla q_{\parallel} - q_{\parallel}\mathbf{b}\cdot\nabla \ln B - Q\right]$$
$$+\frac{2}{3eB}s^2\left(\frac{3}{2}\xi^2 - \frac{1}{2}\right)\left[\left(\frac{5}{2} - s^2\right)\left(\nabla \ln B - 2\kappa\right) + \nabla \ln n\right]\cdot\nabla T\times\mathbf{b}$$
$$+\frac{4}{3eB}\left(\frac{s^4}{2} - \frac{5}{2}s^2 + \frac{15}{8}\right)\left(\nabla \ln B + \kappa\right)\cdot\nabla T\times\mathbf{b}]f_{\rm M}.$$

The red and blue terms couple the entire velocity space grid. We note that the blue terms involve moments of f_{NM}, which is the quantity being advanced. We implemented these terms in a fully implicit fashion in the NIMROD integrand (*dot*) routine that computes the nonlinear matrix vector product. This implicitness is helpful in stabilizing the simultaneous F/T advance described above. The black terms are parameterized by normalized speed, s, hence, they are exactly preconditioned by the diagonal-in-s scheme that has been developed using SuperLU[13], the direct sparse solver NIMROD employs to invert its preconditioning matrices. We note that we have implemented the same CEL-DKE in NIMROD for electrons and ions. The higher-order corrections for finite-orbit-width effects for the ions have not been implemented. Nevertheless, the conservation properties of the CEL method and a correct account of the dominant parallel dynamics has been verified for both thermal electrons and ions.

In order to understand 4D numerical simulations involving the coupled CEL-DKE/NIMROD-fluid system, we implemented probes that tracked the Maxwellian moments of the kinetic distortion (non-Maxwellian) as a function of time throughout NIMROD's domain. This CTTS effort identified rapid growth of Maxwellian moments over short time scales, a feedback effect that is tied to undamped elements in the null space of the CEL-DKE operator. Figure 5 shows NIMROD's poloidal FE grid (left) for a high aspect ratio case that was used to diagnose the coupled fluid/kinetic time advance. The probe locations (dots) shown on the right are where we monitored the Maxwellian moments of f_{NM}.

We reference the time $t = 0.5ms$ in the *qpi* (parallel ion heat flow) plot in Fig. 6. Without using a technique to suppress Maxwellian moments in f_{NMi}, the simulation (here the parallel ion heat flow moment of f_{NMi} blows up rapidly around $t = 0.5ms$. In this simulation, we are evolving the full fluid system, which allows poloidal and toroidal flows and heat flows to develop while density and the temperatures relax slowly on perpendicular transport time scales. The Maxwellian moment suppression in f_{NM} is what permits stable evolution to a nearly time-asymptotic state with slow (transport) evolution governed by small, perpendicular particle, momentum and heat diffusivities. Evolution to a 4D, hybrid fluid/kinetic steady-state with self-consistent closures $q_{\parallel i}$ (left) and the associated f_{NMi} (right) has been an important development funded by the CTTS effort at USU.

The collaboration between NIMROD CDK developers, Drs. Held and Spencer at USU and Joseph Jepson at UW-Madison has led to the first comprehensive, hybrid fluid/kinetic implementation of the Chapman-Enskog-like method in a plasma fluid code. This effort is summarized in the following two publications:

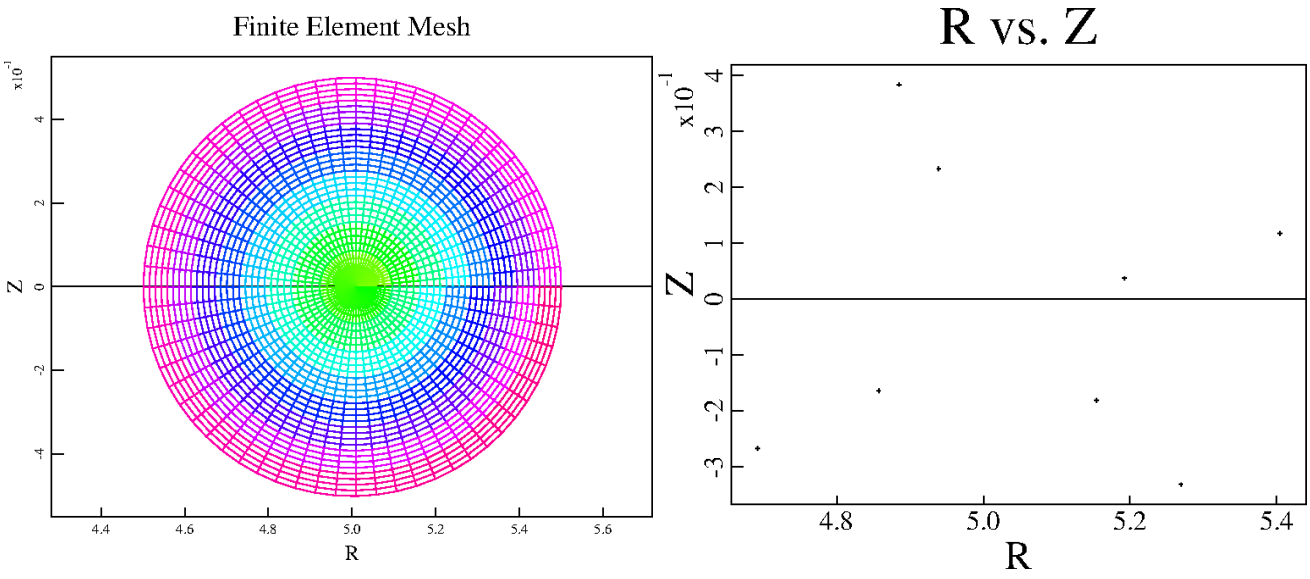

Figure 5: NIMROD's 2D, poloidal plane FE grid for a high aspect ratio test case involving the fully coupled ion CEL-DKE/NIMROD system. Probe locations (right) show where Maxwellian moments of f_{NM} are being monitored during the simulation.

J. R. Jepson, C. C. Hegna, E. D. Held, J. A. Spencer and B. C. Lyons, "Benchmarking NIMROD continuum kinetic formulations through the steady-state poloidal flow", *Phys. Plasmas*, **28**, 082503 (2021),

and

Joseph R. Jepson, Chris C. Hegna, Eric D. Held, Carl R. Sovinec, J. Andrew Spencer, Eric C. Howell, "An analysis and successful benchmarking of the Chapman-Enskog-like (CEL) continuum kinetic closure approach algorithm in NIMROD", *submitted to Computer Physics Communications in January 2024*.

These papers show the value of the Chapman-Enskog-like hybrid fluid/kinetic model that has been implemented in NIMROD. They also highlight the collaborative nature of NIMROD with researchers from several universities (Held, Spencer and Adair at USU and Sovinec, Hegna, and Jepson at UW-Madison) and companies (General Atomics, B. C. Lyons) and TECH-X (E. C. Howell) working together to make NIMROD a valuable tool for the MFE community.

4.2 Port of NIMROD CDK preconditioners to GPUs

The deployment of self-consistent CDK/MHD simulation capability in NIMROD requires an extraordinary amount of compute power. To meet this challenge and adapt to a changing supercomputing landscape, USU is focused on adopting new strategies that harness the power of GPUs, together with distributed-memory multi-core and shared-memory architectures. In loose collaboration with CTTS, a handful of NIMROD developers at other institutions have rewritten its core integrand routines using OpenACC to optimize the heterogeneous parallelism for effective use of GPUs[14].

We extended USU's CTTS effort in this area by exploring the offloading CDK preconditioning onto the GPUs. As mentioned previously, effective physics-based preconditioning for the extremely large linear systems that arise from discretizing the CDK equation is essential to rapid convergence of the

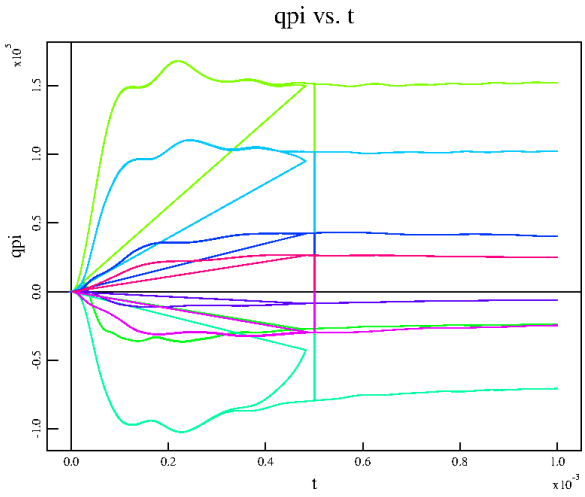

Figure 6: Without suppression of Maxwellian moments in f_{NMi}, the 4D coupled fluid/kinetic simulation undergoes numerical instability around $t = 0.5$ ms as seen in the ion parallel heat flow probe. With Maxwellian moments numerically suppressed, evolution to the nearly steady state is acheived.

core solver. To get started down this path, USU participated with a group of NIMROD developers in the NERSC (July 2020) and OLCF (October 2020) GPU Hackathons. USU's focus was offloading the task of inverting CDK preconditioning matrices using GPU-enabled sparse matrix solvers[15, 16]. GPU-enabled SuperLU_DIST [17, 13] was used in the first hackathon and GPU-enabled Ginko [18, 19] in the second. Figure 7 shows that in both cases, we succeeded in effectively utilizing the GPUs and greatly reducing computation time. The points labeled SLU CPU use only the multi-core functionality of SuperLU_DIST. The points labeled SLU+GPU assign one GPU to each CPU. The points labeled SLU+GPU+OMP additionally utilize shared memory and processor sets within each node. While we were able to find a set of parameters for Ginkgo that made the computation time faster than SuperLU_DIST, Ginkgo can only operate on a single node (single processor) with a single GPU.

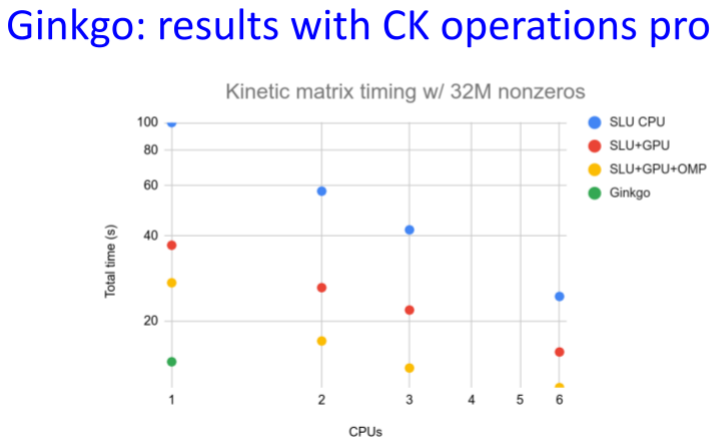

Figure 7: Results from Hackathon tests of solvers on GPUs with CDK matrices.

Sparse matrix solver algorithms are challenging to implement on GPUs because frequent com-

munication patterns are required. The plan that emerged from these two hackathons is to maintain flexibility in leveraging external GPU-enabled codes to invert CDK preconditioning matrices. Other GPU-enabled linear algebra solvers include SuiteSparse 4.6.0 BETA [20, 21, 22], a suite of sparse matrix algorithms with multi-GPU functionality, and MAGMA [23, 24], a dense linear algebra library for heterogeneous/hybrid architectures starting with Multicore+GPU systems. cuSOLVER [25], a direct solver from Nvidia that uses real data types, was also partially implemented during the hackathons, but requires converting NIMROD's complex system to real data types.

Flexibility in leveraging external codes is crucial for efficient CDK preconditioning. Direct solvers like SuperLU_DIST and cuSOLVER may not provide the optimal strategy. Often in NIMROD the preconditioning solve only needs to be approximate. This flexibility will allow us to test many solvers within the larger context of the full algorithm. Once the test code is ported to the full application, different solvers and strategies can be tested. For example, the iterative solve in Ginkgo may improve with a better initial guess for the solution. The testing of polynomial extrapolation for an initial guess will be examined in the context of the full NIMROD code.

5 Expanded continuum drift kinetic (CDK) RE capability in NIMROD

Funded CTTS work at USU has led to a CDK implementation for runaway electrons (REs) in NIMROD that includes advection with parallel streaming and $\mathbf{E} \times \mathbf{B}$ drifting, particle trapping, $\mathbf{E}$ acceleration along $\mathbf{B}$, sychrotron radiation and the fully relativistic, test particle operator[26]. All of this physics was implemented using a fully implicit time step normalized to the relativistic collision time, $\tau = 4\pi\epsilon_0^2 m_e^2 c^3/(ne^4 \ln\Lambda)$. While this allows for large time steps, it also couples all of the degrees of freedom (dofs) in the 2D relativistic phase space, thus placing a huge demand on effective, physics-based preconditioning.

Fluid models of REs[27, 28] often use Dreicer[29, 30] and avalanche[31] mechanisms as sources for the RE fluid density, n_{RE}. The RE fluid velocity[27], $\mathbf{v}_{RE} = fc\mathbf{B}/B + \mathbf{E} \times \mathbf{B}/B^2$, and current, $\mathbf{j}_{RE} = -en_{RE}\mathbf{v}_{RE}$, then complete the set of closures for the fluid model. RE fluid models use the coefficient f in $\mathbf{v}_{RE}$ to reduce time step constraints with the requirement that fc is kept large compared to the Alfven time[27]. For the CDK RE equation, however, NIMROD solves at a set of collocation points in p. This emphasizes the need for a fully implicit time advance.

In the CDK RE equation, the RE sourcing mechanism is contained in the balance between $\mathbf{E}$-acceleration, synchrotron radiation and the relativistic collision operator. Figure [**?**] shows RE distribution function contours resulting from a 2D phase space simulation that Tyler Markham did using NIMROD. Figure 8 was taken from the thesis

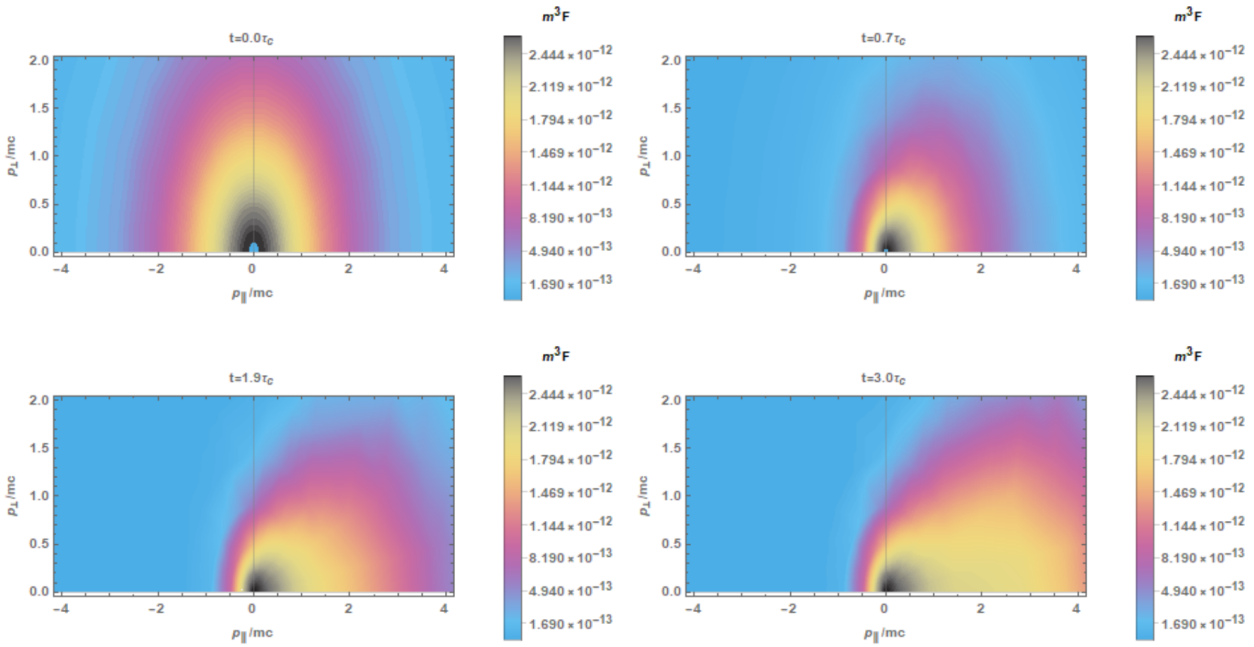

Figure 8: Evolution of an unshifted Maxwell-Jüttner distribution over 30 normalized time-steps $\Delta t = 0.1$ with $\mathbf{E}$-acceleration ($E_{||} = 2.25$ times the Conner-Hastie field), synchrotron radiation, and the relativistic, linearized collision operator.

Relativistic, Continuum Drift-Kinetic Capability in the NIMROD Plasma Fluid Code"[3], PhD thesis defended in December 2022 (Available at `https://digitalcommons.usu.edu/etd/8683/`)

which exercised NIMROD's existing RE capability and included a preliminary implementation of

the nonlinear, relativistic Braams-Karney collision operator. After graduating, Tyler moved on to a postdoc at Los Alamos National Lab.

Since the CDK RE equation is to be solved throughout NIMROD's spatial domain as well as in the 2D phase-space (p, ξ), closures are computed as integrals of the evolving RE distribution

$$\{n_{RE}, \mathbf{j}_{RE}\} = \frac{2\pi}{m^3} \int_{-1}^{1} d\xi \int_{0}^{\infty} p^2 dp \{1, -e\mathbf{v}_{\rm gc}\} F_{RE}(\mathbf{x}, t, p, \xi). \tag{7}$$

Our plan is to extend $\mathbf{v}_{gc}$ to the full form for the relativistic guiding center drift given in Ref. [32]. Future emphasis for CDK RE will be on a self-consistent, tight coupling of 5D RE physics into NIMROD's fluid model to allow for comparison with the fluid RE results and exploration of the effects of the relativistic phase space dynamics.

6 Serendipity shape functions for NIMROD's PIC algorithm

Finally, funded CTTS work at USU led to improvements in NIMROD's PIC algortihm, which was pioneered by Dr. Charlson Kim. The goal was to use higher-order (than bilinear) functions in the particle search algorithm and field (R, Z, $\mathbf{B}$, ...) evaluations. One useful set for this purpose is the serendipity shape functions, the middle two nodal sets shown in Fig. 9 are two examples. Aspects of higher-order convergence in trajectories (R and Z) and velocity components ($v_\parallel$) and savings in wallclock time and memory were four successful outcomes of this effort.

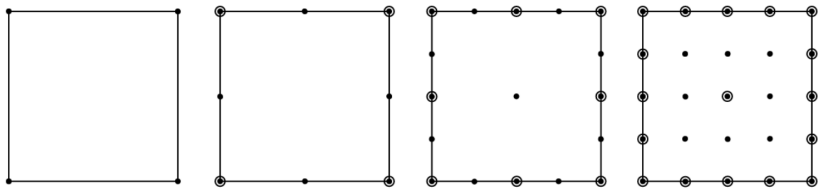

Figure 9: From left to right, the nodal representations are: bilinear, serendipity biquadratic, serendipity biquartic and 2D Lagrange biquartic (exact). NIMROD's coordinates, R and Z, and fields are expanded using all of the nodes (dots) on the far right for the biquartic case. The middle two serendipity nodal sets retain higher order while providing savings in the particle push and find times as well as memory.

Figure 10 shows error in the parallel component of the PIC particle velocity averaged over 30,000 particles for various serendipity nodal sets. Here error is computed against those of "exact" trajectories computed using the full 2D Lagrange polynomial basis and sixth-order 1D polynomials. Going beyond biquartic is not helpful. However, biquartic with the center node further reduces the error. The data were computed at timestep 35, 350 and 3500.

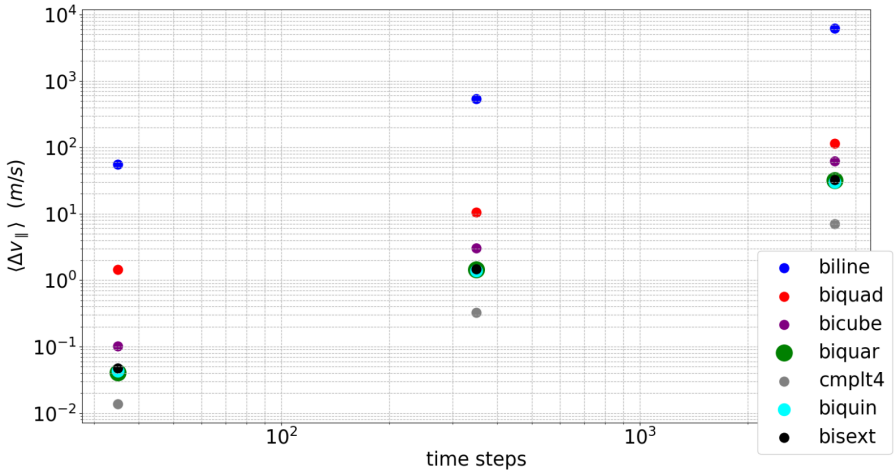

Figure 10: Errors in $v_\parallel$ averaged over 30,0000 markers show a sweet spot when using the biquartic (cmplt4) serendpity nodal sets with the extra node in the middle (third cell in Fig. 9).

Part of this effort also led to the implementation of global structures for R, Z, and field quantities which allowed processors to push PIC particles throughout NIMROD's domain without having to hand them off when crossing block boundaries. This led to improved load balancing and reduced push time for the particles. For the same 3500 timestep case (right) shown in Fig. 10, run times and memory for

the various representation are shown. We highlight the improvements offered by the cmplt4 (serendipity biquartic with a center node) in the polynomial degree 4 column of Figs. 11 and 12. This work

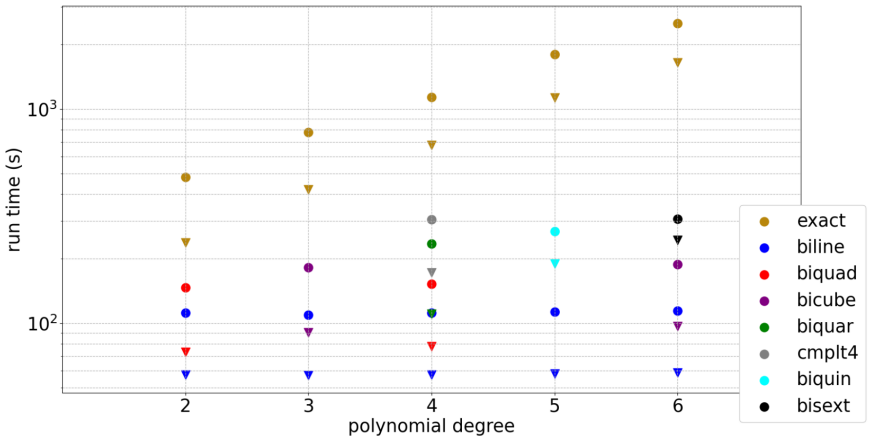

Figure 11: The polynomial degree=4 column shows a factor of 5 reduction in runtime when using the cmplt4 serendipity basis versus the full 2D Lagrange polynomials. The considerable reduction in error for the cmplt4 basis is seen compared to NIMROD's usual bilinear search and field routines in FIg. 10

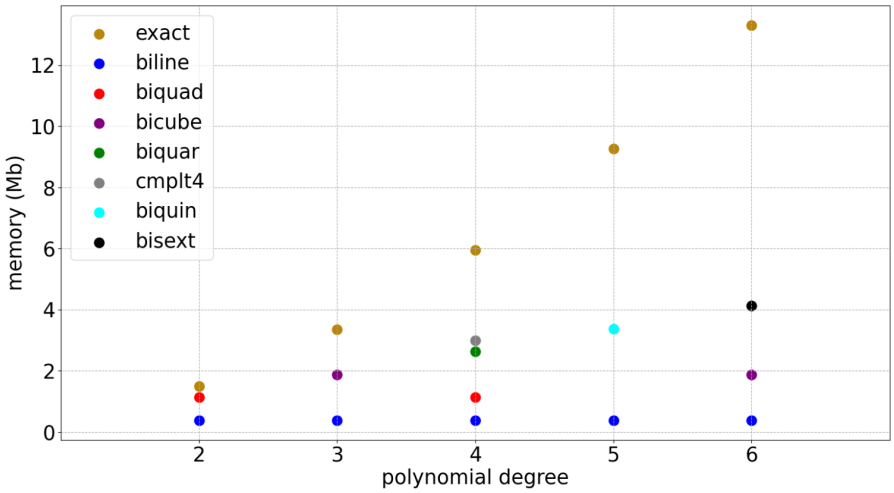

Figure 12: The polynomial degree=4 column shows a factor of 2 reduction in memory when using the cmplt4 serendipity basis versus the full 2D Lagrange polynomials.

was summarized in Trevor Taylor's PhD thesis

Serendipity Shape Function for Hybrid Fluid/Kinetic-PIC Simulation[5], PhD thesis defended in October 2022 (Available at `https://digitalcommons.usu.edu/etd/8652/`).

Importantly, this version of the PIC particles is being used by ORNL in its effort to implement a KORC/NIMROD coupling.

7 Educational Opportunities

Three PhD students, Trevor Taylor (PhD October 2022), Tyler Markham (PhD, December 2022) and Hankyu Lee (PhD, expected May 2024), were partially supported as research assistants (RAs) using USU CTTS funds. A final student, Brett Adair also received CTTS funding to help with improvements to the Rosenbluth potential implementation in NIMROD.

Trevor Taylor's PhD thesis, "Serendipity Shape Function for Hybrid Fluid/Kinetic-PIC Simulation", extended NIMROD's bilinear search and field evaluation routines in its PIC capability to include higher-order basis functions. The serendipity set allowed for higher accuracy while reducing memory since it ignores interior node points in NIMROD's 2D finite-element representation for the poloidal plane.

Tyler Markham PhD thesis, "Relativistic, Continuum Drift-Kinetic Capability in the NIMROD Plasma Fluid Code", presented 2D relativistic phase space results for NIMROD's CDK runaway electron (RE) model and described the implementation of the fully nonlinear, relativistic Braams-Karney collision operator. This thesis has laid the groundwork for full 4D and 5D CDK-RE/NIMROD-MHD studies of REs during tokamak disruptions.

Finally, Hankyu Lee has been working on implementing Dr. Ji's moment method for closures in NIMROD. This effort was based on the existing CDK implementation, hence rapid progress was possible by adopting a similar algorithmic approach. Hankyu will defend his PhD in May of 2024.

Each of these students did a good job learning plasma theory and computation under the supervision of Drs. Held, Spencer and Ji at USU. Our plasma fusion group was able to expand thanks to CTTS funds. The Physics Department at USU appreciated that growth and the vibrant group that we have developed.

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