

An Improved Equation-Free Projective Integration Method for Gyrokinetic Profile Evolution of Tokamak Plasmas

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Outline:



- 1 Introduction
- 2 Numerical Approach
- 3 Verification in XGCa
- 4 Summary and Outlook

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- 1 Introduction
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- ▶ Relevant physical processes in magnetically confined fusion plasmas can be strongly coupled across multiple scales :
 - Cross-field transport from micro-turbulence, neoclassical orbital dynamics, collisions, etc. causes slow evolution of macroscopic profiles in a tokamak.
 - Macroscopic profiles drive collisional neoclassical orbit motions and micro-turbulence evolving on small spatial and/or temporal scales.
- ▶ Full- f gyrokinetics captures these interactions self-consistently, but a direct time-stepping approach to transport time scales is not practical due to computational resource requirements.
- ▶ Error accumulation in long-time simulations presents an additional problem.
- ▶ Fast timescale physics (turbulence, orbital dynamics, etc.) is **dynamically-relevant** → cannot “step over” with traditional implicit schemes.
- ▶ Algorithmic and modeling innovation is required.

- ▶ Traditionally, gyrokinetic simulations take profiles as an input and focus on cross-field fluxes as output; short timescale simulations (order of ms).
- ▶ Profile prediction as an inverse problem : sources (e.g. heating, torque) as input, profiles as output → requires much longer time simulations
- ▶ Previous and ongoing efforts:
 - TGYRO
 - ▶ J. Candy, C. Holland, et al, Phys. Plasmas **16**, 060704 (2009)
 - ▶ Newton's method for iteratively adjusting 1D steady-state profiles to achieve power balance in local flux-tube simulations
 - TRINITY
 - ▶ M. Barnes, I. G. Abel, et al, Phys. Plasmas **17**, 056109 (2010)
 - ▶ Couples local flux-tube simulations to implicitly discretized 1D transport model; allows time-evolving profiles
 - TANGO
 - ▶ J. Parker, L. LoDestro, et al, Nucl. Fusion **58**, 054004 (2018)
 - ▶ Couples global gyrokinetic simulations to 1D transport model; Picard iteration (LoDestro method)

Philosophy for Equation-Free Modeling:

Use appropriately initialized micro-scale simulations over short time intervals to make long-time predictions of macro-scale behaviors.

- ▶ Yes, we use equations (it's not magic).
- ▶ However, we only have equations on the micro-scale (gyrokinetics). We bypass the derivation of macro-scale (transport) equations.
- ▶ There are analogies to matrix-free methods in numerical linear algebra.

Equation-free projective integration for kinetic plasma simulation :

- ▶ M. Shay, J. F. Drake, and B. Dorland, J. Comput. Phys. **226**, 571-585 (2007)
- ▶ P. Cazeaux and J. Hesthaven, arXiv:1610.01071v1, (2016)
- ▶ D. Green and S. DePascuale (Dynamic Mode Decomposition)
- ▶ B. Sturdevant, S. Parker, R. Hager, and C.S. Chang, to appear in Phy. Plasmas (2020)

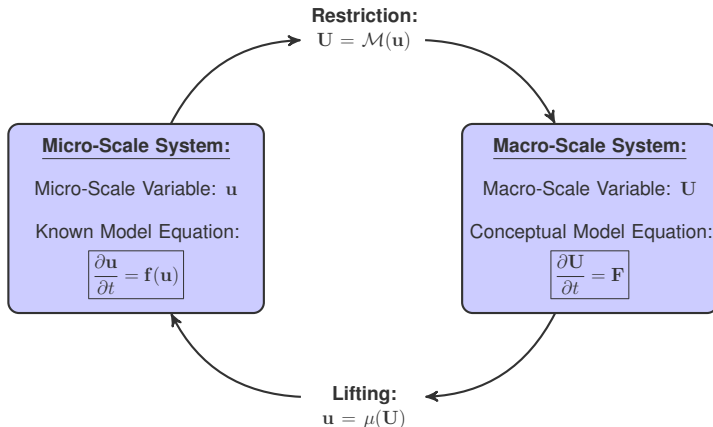
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Equation Free Modeling

Micro-Scale and Macro-Scale Systems

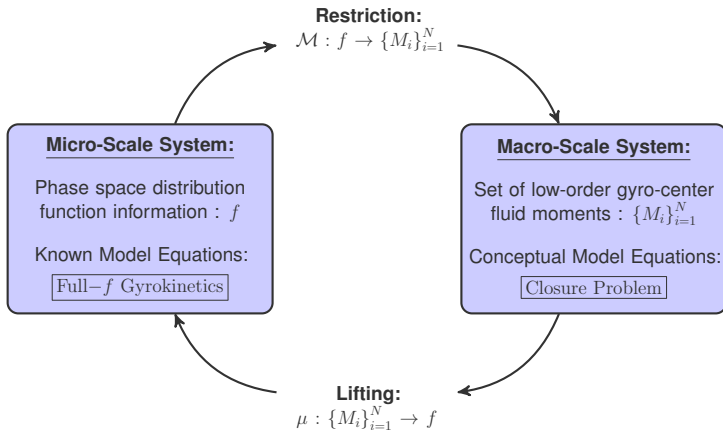


C. W. Gear and I. G. Kevrekidis, SIAM J. Sci. Comp., 24(4) (2003)

C. W. Gear et. al., Comm. Math. Sci., 1(4), 715-762 (2003)

Equation Free Modeling

Application to Kinetic Models



Similar approach considered previously in:

M.A. Shay, J.F. Drake, B. Dorland, Journal Comput. Phys., 226, (2007).

A Maxwellian was assumed in the lifting operator.

Equation Free Modeling

Macro-scale Variable and Restriction Operator



- Choose a finite dimensional linear space of multi-variate polynomials in $\mathbf{v}$:

$$\mathbb{P} = \left\{ \sum_{\mathbf{j} \in \mathcal{S}} a_{\mathbf{j}} \mathbf{v}^{\mathbf{j}} \mid a_{\mathbf{j}} \in \mathbb{R} \right\}$$

- $\mathbf{j} = (j_1, j_2, \dots, j_d)$, $\mathbf{v}^{\mathbf{j}} = v^{j_1} v^{j_2} \dots v^{j_d}$, d : number of velocity coordinates, $\mathcal{S}$: set of multi-indices with $|\mathcal{S}| = \dim(\mathbb{P}) \equiv N < \infty$.
- Choose a basis for $\mathbb{P}$: $\{\Psi_i\}_{i=1}^N$
- Restriction operator is a set of functionals $\{G_i\}_{i=1}^N$ mapping a phase space distribution function $f(\mathbf{x}, \mathbf{v})$ to a fluid moment M_i .

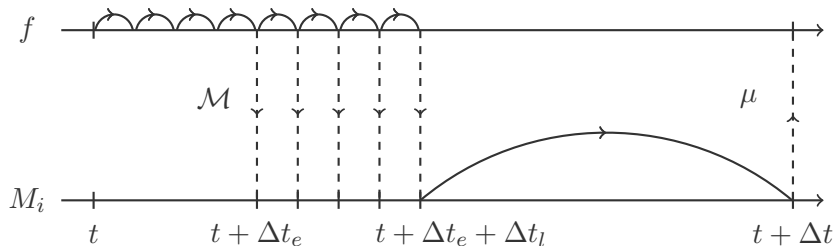
$$G_i[f] = \int_{\mathbf{v}} f \Psi_i d\mathbf{v}$$

- The macro-scale variable $\mathbf{U}$ is the set of N fluid moments $\{M_i\}_{i=1}^N$, obtained by applying each G_i to f .

$$M_i = G_i[f]$$

Projective Integration

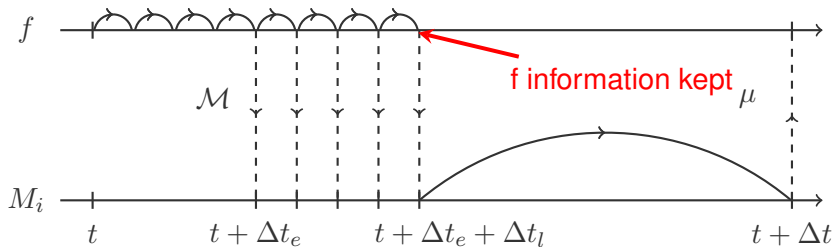
Linear Least Squares Projective Integrator (Known Method)



- ▶ Simulate for Δt_e to allow system to equilibrate or "heal" (some disturbance from lifting)
- ▶ Simulate additional Δt_l , restricting over several time steps to get a short time history of M_i
- ▶ Take a linear least squares fitting in time and project M_i to $t + \Delta t$
- ▶ Apply a lifting operator to continue at next projective time step (Key!)

Projective Integration

Linear Least Squares Projective Integrator (New Lifting)



- ▶ Simulate for Δt_e to allow system to equilibrate or "heal" (some disturbance from lifting)
- ▶ Simulate additional Δt_l , restricting over several time steps to get a short time history of M_i
- ▶ Take a linear least squares fitting in time and project M_i to $t + \Delta t$
- ▶ Apply a lifting operator to continue at next projective time step (Key!)

Improved Equation Free Modeling

Kinetically-Informed Lifting Operator



- ▶ To take multiple projective time steps, a "lifting operator" is necessary which maps the macro-scale variable to the micro-scale variable.

Lifting Operator:

There is not enough information in the macro-scale state to uniquely determine a micro-scale state. Additional constraints must be chosen carefully to preserve the long time-scale dynamics.

- ▶ Our approach is to reuse as much available kinetic information as possible.
- ▶ We have known distribution function information from before projective step. Take the lifted distribution function as :

$$f_{new}(\mathbf{x}, \mathbf{v}) = \mathcal{T}(\mathbf{v}, \boldsymbol{\alpha}) f_{old}(\mathbf{x}, \mathbf{v}),$$

where we choose a form for $\mathcal{T}$ depending on N parameters $\boldsymbol{\alpha}$.

- ▶ Requiring f_{new} to match the projected moments gives N constraints used to determine $\boldsymbol{\alpha}$:

$$M_i(\mathbf{x}) = G_i[\mathcal{T}(\mathbf{v}, \boldsymbol{\alpha}) f_{old}(\mathbf{x}, \mathbf{v})], \quad \text{for } i = 1, \dots, N$$

- ▶ Preserves structure of higher order moments.

Improved Equation Free Modeling

Polynomial Transformation Lifting Operator



- Choose a basis for $\mathbb{P}$: $\{\varphi_j\}_{j=1}^N$ and expand $\mathcal{T}$ and Ψ_i :

$$\mathcal{T} = \sum_j \alpha_j \varphi_j, \quad \Psi_i = \sum_j s_{i,j} \varphi_j, \quad \alpha_j, s_{i,j} \in \mathbb{R}$$

- Plugging expansions into the moment constraints yields a linear system of N equations for the N unknowns $\{\alpha_i\}_{i=1}^N$

$$A \underline{\alpha} = S^{-1} \underline{\mathbf{m}}$$
$$A_{i,j} = \langle \varphi_i, \varphi_j \rangle, \quad \underline{\alpha}_j = \alpha_j, \quad \underline{\mathbf{m}}_i = M_i, \quad S_{i,j} = s_{i,j}$$

- Since $f_{old} \geq 0$, we can define a weighted inner product $\langle \cdot, \cdot \rangle : \mathbb{P} \times \mathbb{P} \rightarrow \mathbb{R}$

$$\langle u, v \rangle = \int_{\mathbf{v}} uv f_{old} d\mathbf{v}, \quad u, v \in \mathbb{P}$$

- Requires a small $N \times N$ matrix inversion for each node.

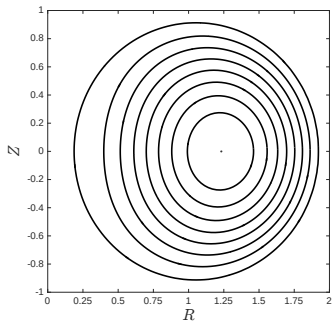
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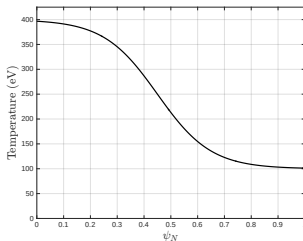
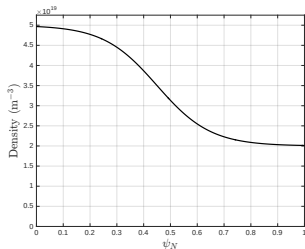
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Verification Problem in XGCa

Neoclassical Ion Heat Transport

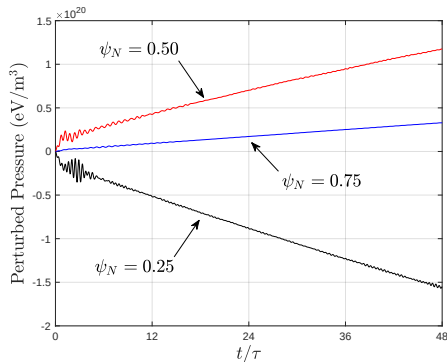
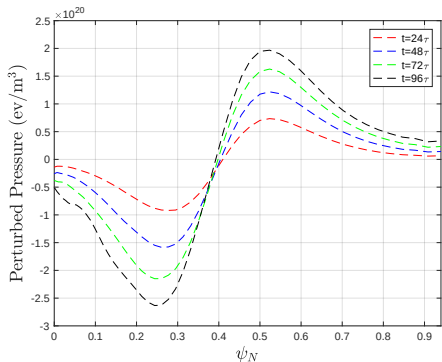


- ▶ Circular plasma boundary, shifted magnetic geometry
- ▶ Initial background density and temperature profiles
- ▶ $n_i = n_e$ and $T_i = T_e$
- ▶ Gyrokinetic ions, adiabatic electrons.
- ▶ Verify macroscopic T_i profile relaxation due to microscopic neoclassical ion orbits and Coulomb collisions.



Verification Problem in XGCa

XGCa Reference Solution



Running XGCa for this model, we obtain a reference solution to which we can compare the results of the equation-free projective integration method.

- ▶ Fast time scale : neoclassical ion orbits, Coulomb collisions, damped oscillations from Geodesic Acoustic Modes (GAMS).
- ▶ Slow time scale : quasi-steady state evolution of a slowly growing pressure perturbation to flatten pressure profile.

Verification Problem in XGCa

Model Equations



- ▶ Gyrokinetic equation for ion guiding center distribution function:

$$\frac{\partial f_i}{\partial t} + \dot{\mathbf{X}} \cdot \frac{\partial f_i}{\partial \mathbf{X}} + \dot{v}_{\parallel} \frac{\partial f_i}{\partial v_{\parallel}} = C_{ii}(f_i; f'_i)$$

- ▶ Quasi-neutrality:

$$-q_i n_i^{pol}(\phi) + e n_e(\phi) = q_i \bar{n}_i, \quad n_i^{pol}(\phi) = \nabla_{\perp} \cdot \left(\frac{n_0 m_i}{q_i B^2} \nabla_{\perp} \phi \right)$$

- ▶ Adiabatic electrons:

$$n_e(\phi) = n_0 \left(1 + \frac{e(\phi - \langle \phi \rangle)}{T_e} \right)$$

Basis polynomials and macro-scale variables:

$$\Psi_{p,q} = \left(\sqrt{\frac{m_i}{T_i}} v_{\parallel} \right)^p \left(\frac{m_i}{T_i} \mu B \right)^q$$

$$M_{p,q} = \int_0^{\infty} \int_{-\infty}^{\infty} \Psi_{p,q} f B dv_{\parallel} d\mu$$

$$(p, q) \in \{(0, 0), (1, 0), (2, 0), (0, 1)\}$$

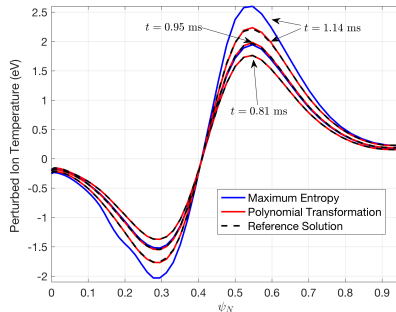
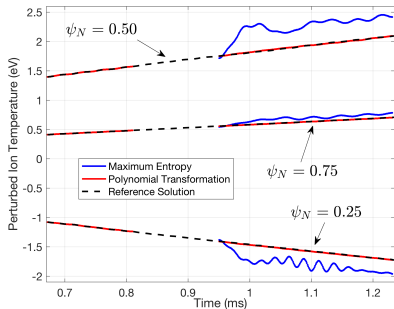
Numerical Studies

Testing the Improved Lifting Operator



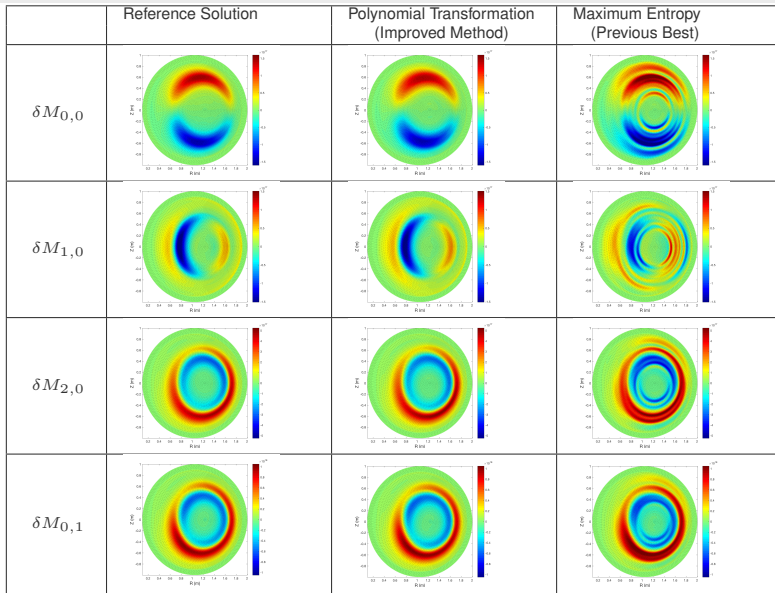
- ▶ Take a "small" projective time step and lift to a new distribution function.
- ▶ Comparisons are made with a lifting operator based on maximum entropy (shifted Maxwellian) constraints for supplying missing information.

$$\delta t = 1.12 \times 10^{-4} \text{ ms}, \quad \Delta t_e = 0.00 \text{ ms}, \quad \Delta t_l = 0.140 \text{ ms}, \quad \Delta t = 0.280 \text{ ms}$$



Numerical Studies

Snapshots at $t = 1.14$ ms



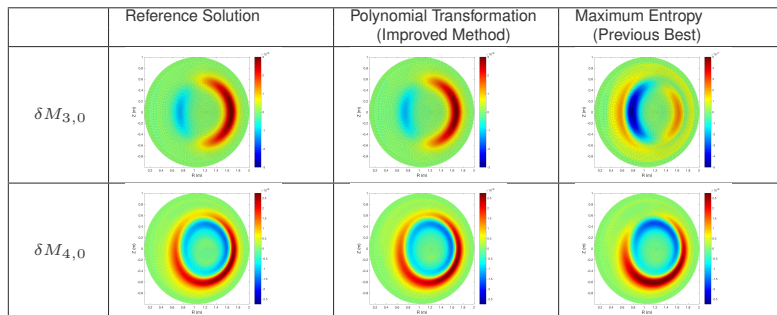
An Improved Equation-Free Method

Numerical Studies

Snapshots at $t = 0.95$ ms



- ▶ Polynomial transformation carries over higher order moment information from previous time step that wasn't explicitly enforced.
- ▶ Maximum entropy (shifted Maxwellian) produces incorrect structure.
- ▶ For example :



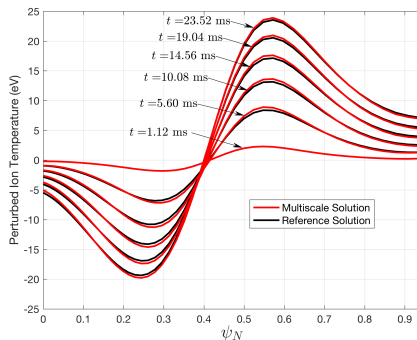
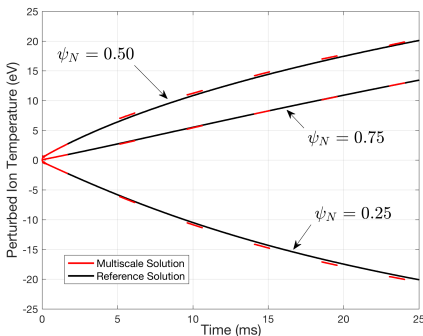
Numerical Studies (Improved Method)

Multiple Projective Steps : Ion temperature perturbation



► Simulation parameters:

$$\delta t = 1.12 \times 10^{-4} \text{ ms}, \quad \Delta t_e = 0.45 \text{ ms}, \quad \Delta t_l = 0.56 \text{ ms}, \quad \Delta t = 4.48 \text{ ms}.$$



- Reduction in number of micro time steps: $\frac{\Delta t}{\Delta t_e + \Delta t_l} = 4.4$ (comparable to computational speedup)
- Temperature **perturbation** stays within 2.5% of reference solution

Numerical Studies (Improved Method)

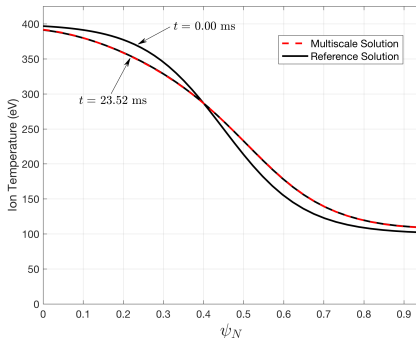
Ion temperature profile prediction



- ▶ Initial and final ion temperature profiles

- ▶ Simulation parameters:

$$\delta t = 1.12 \times 10^{-4} \text{ ms}, \quad \Delta t_e = 0.45 \text{ ms}, \quad \Delta t_i = 0.56 \text{ ms}, \quad \Delta t = 4.48 \text{ ms}.$$



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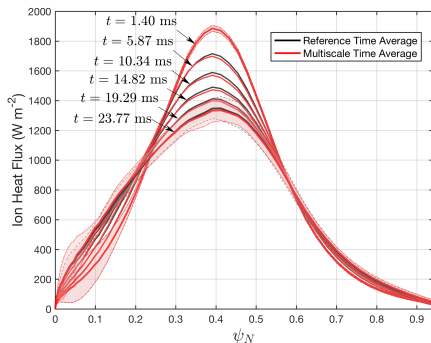
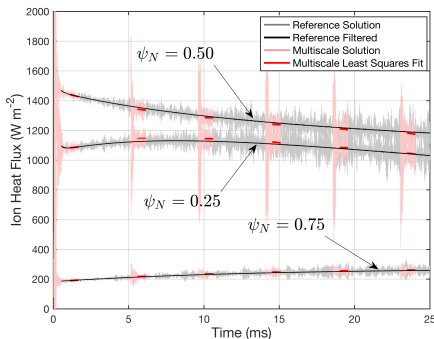
Numerical Studies (Improved Method)

Multiple Projective Steps : Ion heat flux



► Simulation parameters:

$$\delta t = 1.12 \times 10^{-4} \text{ ms}, \quad \Delta t_e = 0.45 \text{ ms}, \quad \Delta t_l = 0.56 \text{ ms}, \quad \Delta t = 4.48 \text{ ms}.$$



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Numerical Properties

Accuracy



Sources of Error :

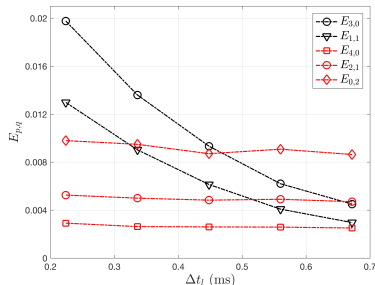
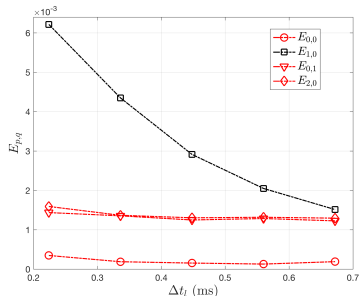
- ▶ Error in micro-simulations
- ▶ Error due to lifting
- ▶ Error due to projective integrator :
 - Estimation of $\frac{\partial \mathbf{U}}{\partial t}$ (controlled by Δt_l)
 - Truncation error (controlled by Δt)

Relative error for moment $M_{p,q}$:

$$E_{p,q} = \frac{\|M_{p,q} - M_{p,q}^{ref}\|_2}{\|\tilde{M}_{p,q}^{ref}\|_2}$$

Fixed Parameters :

$$\Delta t_e = 0.45\text{ms} \quad \Delta t = 4.48\text{ms}$$



Numerical Properties

Accuracy



Sources of Error :

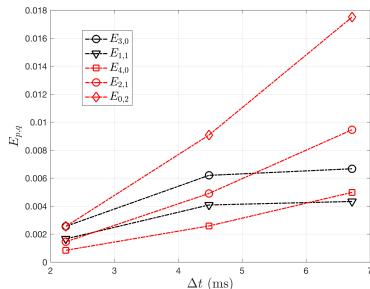
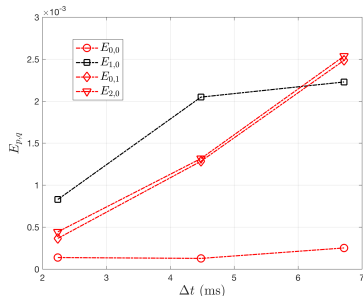
- ▶ Error in micro-simulations
- ▶ Error due to lifting
- ▶ Error due to projective integrator :
 - Estimation of $\frac{\partial \mathbf{U}}{\partial t}$ (controlled by Δt_l)
 - **Truncation error (controlled by Δt)**

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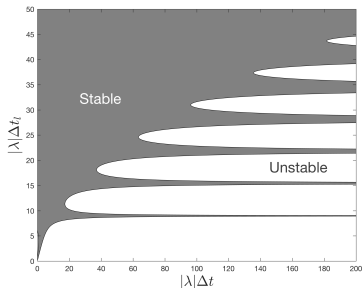
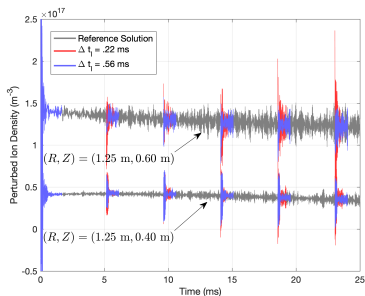


Numerical Properties

Stability : Error Amplification From Oscillations



- ▶ Least squares projective integrator introduces numerical errors at each projective cycle.
- ▶ Solution is displaced from the slow manifold $\rightarrow$ leads to excitation of GAMs in XGC.
- ▶ Analysis shows errors can add coherently, leading to a numerical instability.



- ▶ Avoiding this often requires either XGC to be run over large time intervals or Δt to be small, limiting the computational gains achieved.

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- ▶ A method for applying equation free projective integration to kinetic plasma simulation has been developed.
- ▶ Key to this work was the development of a new lifting operator.
- ▶ Promising initial results for reducing the number of micro time steps needed while accurately reproducing profile evolution

Algorithmic Outlook :

- ▶ Possible improvements to integration scheme:
 - Iterate to return to manifold after projection :
 - ▶ G. Ariel, J.M. Sanz-Serna, and R. Tsai, Multiscale Model. Simul. 10(4), 1180-1203 (2012)
 - ▶ C. W. Gear et al., SIAM J. Appl. Dyn. Syst., 4(3), 711-732 (2006)
 - Improved projective integrators : predictor-corrector with iterative refinement, adaptive time stepping
 - Dynamic Mode Decomposition (being explored by D. Green and S. De Pascuale at ORNL)
- ▶ Exploration of scaling factors to preserve positivity (exponential of polynomial)
- ▶ Opportunities for machine learning

Summary and Outlook

Iterative Predictor-Corrector Method to Improve Stability



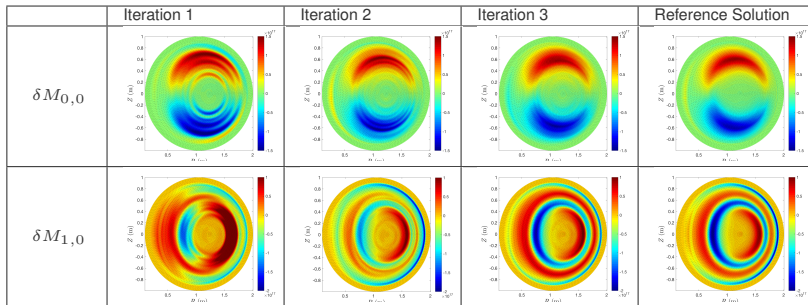
► Simulation Parameters:

$$\delta t = 1.12 \times 10^{-4} \text{ ms}, \quad \Delta t_e = .11 \text{ ms}, \quad \Delta t_l = .22 \text{ ms}, \quad \Delta t = 5.04 \text{ ms}, \quad \alpha = 0.4$$

► Possible reduction in number of micro-steps:

$$\frac{\Delta t}{\text{iterations} \times (\Delta t_e + \Delta t_l)} \approx 5 \quad (\text{using 3 iterations})$$

► Snapshots at 5.88 ms :



► Further studies needed

Physics Outlook :

- ▶ Enable long-time XGC simulations (turbulence + neoclassical + neutrals + heat/torque sources and sinks)
 - ▶ Starting to explore application to total- f turbulence + neoclassical + heat source and sink
 - ▶ Use advanced extrapolation techniques (e.g. DMD) and machine learning for real time evolution prediction from experimental data : profile evolution, neoclassical island structure growth, etc.
-

Questions?



Please Ask!

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