Efficient uncertainty quantification in plasma micro-instability simulations with mode transitions

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Dimensionally adaptive sparse grids that use sensitivity-based refinement has been applied to the forward uncertainty quantification of tokamak plasma micro-instability simulations by Farcas et al [1], for an ASDEX Upgrade (AUG) reference shot #33585 [2]. Dimensionally adaptive approaches are generally constructed with basis functions that have global support and are appropriate for target quantities with global smoothness. Here the work of Farcas et al, is continued to investigate spatially adaptive sparse grid approximations for problems where quantities of interest have discontinuities or sharp gradients.

Plasma micro-instability simulations are a key to understanding and optimizing confinement properties of magnetic confinement fusion devices. When validating these simulations against experimental scenarios, the effects of experimental uncertainty for the input parameters must be propagated to establish the corresponding distributions of output quantities of interest. Internal uncertainty propagation through each simulation component is often impractical and non-intrusive techniques that use a set of simulation input-output points is required. For computationally expensive numerical simulations, data efficiency is of paramount importance. A data-efficient technique is to assume a functional form $f(\vec{x})$ between the input points $\vec{x}$ within the uncertainty space. The expectation and variance of the output of interest are then $E\big(f(\vec{x})\big) = \int P(\vec{x}) f(\vec{x}) d\vec{x},\ Var\big(f(\vec{x})\big) = E(f(\vec{x})^2) - E\big(f(\vec{x})\big)^2$. The variance can be used to determine sensitivity information via the Sobol indices $S_i = \frac{Var\left[E\left(f(\vec{x})\middle|x_i\right)\right]}{Var[f(\vec{x})]}$ which is a measure of a parameter's contribution to the output variance and provides insight into the turbulence drives. High dimensional input spaces with discontinuities notoriously require a large amount of simulation points and exploring adaptive methods to select the most informative points must be explored.

Sparse grid methods have been proven to be extremely data efficient across many fields for high dimensional interpolation, integration and solving partial differential equations [3-8]. A surplus based refinement strategy was shown to resolve a discontinuity associated with a micro-instability mode transition [8]. This conference proceeding paper takes this surplus based sparse grid refinement strategy and applies it to the same uncertainty quantification problem explored by Farcas et al. [1]. No hyperparameter tuning was applied; the data efficiency is presented as a baseline for further improvement.

Shot #33585 [2] is a low density, predominantly electron heated L-mode plasma, with a 2.5T on axis magnetic field and 1.0 MA of plasma current. The applied heating was Ohmic and 0.7 MW of Electron Cyclotron Resonance Heating. The simulations are carried out for $\rho_{tor} = 0.75$ and $k_y = 0.6$. The micro-instability simulations are conducted with the Gyrokinetic Electromagnetic Numerical Experiment (GENE) code which has an option to solve the linear versions of the gyrokinetic equations which provides essential information on the transport channel ratios, instability drives and domain resolutions to direct full non-linear simulations that are capable of determining the heat, particle and momentum fluxes [9]. In linear simulations the amplitude of the micro-instability fluctuations grows exponentially with time at some growth-rate. The growth-rate of the dominant instability is the output of interest for this uncertainty quantification study. The dominant instability can change as one scans the input parameter space and this causes the discontinuities that need to be accounted for. The GENE input uncertainties have been obtained via a combination of plasma diagnostic uncertainties and expert opinion derived from the kinetic profiles and magnetic equilibrium (Table 1).

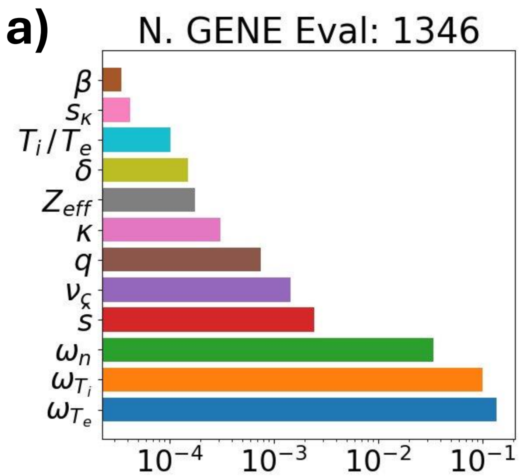
Parameter	Lower	Upper
Equilibrium Elongation Gradient s_κ,	0.208	0.254
Equilibrium Elongation, κ	1.282	1.416
Equilibrium Triangularity, δ	0.053	0.058
Safety Factor, q	2.171	2.399
Magnetic Shear, ŝ	1.993	2.436
Plasma Beta, β	4.89e-04	5.98e-04
Normalised Density Gradient ω_n,	1.156	1.927
Normalised Electron Temperature Gradient ω_{T_e},	4.040	6.734
Normalised Ion Temperature Gradient ω_{T_i},	2.097	3.494
Temperature Ratio, T_i/T_e	0.614	0.679
Collision Frequency ν,	6.41e-04	8.68e-04
Effective Ion Charge Z_{eff},	1.280	1.920

Table 1. Relevant uncertain GENE input parameters considered in this study.

This study uses a spatially adaptive sparse grid that refines the single point with maximum surplus and uses a degree 10 polynomial basis function with local support and no boundary points. The grid is initialised with a level 2 static grid over the 12D space. The specific implementation is the SG++ package and the ModPolyGrid object [8]. Sparse grid points are deterministically selected for a hierarchy of basis functions interpolant $f(\vec{x})$. The interpolant integral can be exactly computed via a quadrature rule and this can be used to efficiently compute the expectation and variance for the interpolant regardless of the dimensionality.

Static sparse grids are optimised for smooth functions with independent inputs and spatially adaptive sparse grids mitigate these assumptions. Sparse grids are constructed in levels, with higher levels having a higher resolution of points. Each point has a polynomial basis function which is modified to only be non-zero in a local region around the point. The surplus is a coefficient for the basis function in the interpolant, which magnitude represents that basis functions contribution to the overall interpolant. The surplus is also an error computed as the difference between the function evaluation and the interpolation from lower levels. If the low-level interpolant has a large error at a point of evaluation it is likely due to a discontinuity or local feature near the point, such that a surplus refinement indicator leads to more points being sampled near discontinuities.

The subsequent Sobol indices sensitivity analysis performed with the sparse grid interpolant indicates that for this scenario the normalised gradients of the kinetic profiles are the most significant sources of uncertainty by orders of magnitude (Fig 1a). This is expected as these are the parameters which drive the observed instability modes, TEM-ITG and ETG; the same result was found in the previous study [1]. Surplus refinement sparse grids sampled heavier along these dimensions and close to the discontinuities (Fig 1b), and thus these methods show potential to provide data efficient uncertainty quantification for discontinuous micro-instability derived functions.



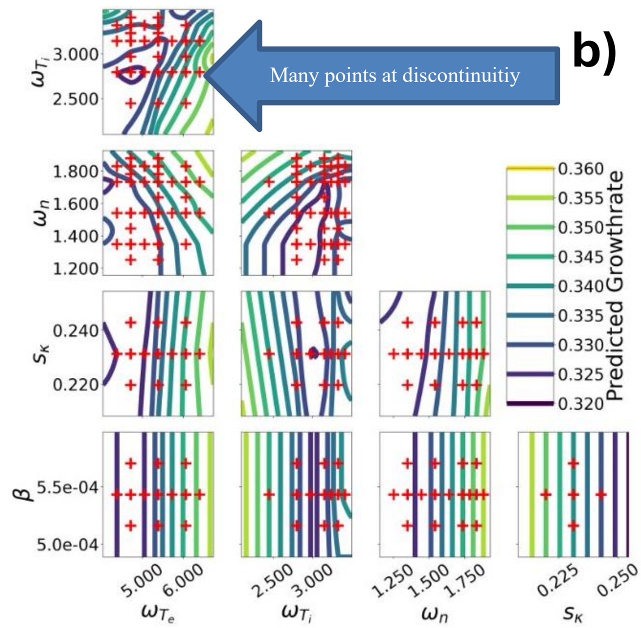


Fig 1a: The first order Sobol indices of the interpolant after 1346 samples, b: 2D slices of the interpolant for the 3 most and 2 least significant parameters with the sparse grid points overlayed.

The data efficiency can be observed via the number of samples required to have an expected value close to the true value. The true expected value is defined as the arithmetic mean from a pseudorandom Sobol sequence that is continually sampled until the arithmetic mean and standard deviation converges within the precision of 10^{-3}. The first attempted surplus based refinement strategy with no hyperparameter tuning, did not achieve a data efficiency required for practical application.

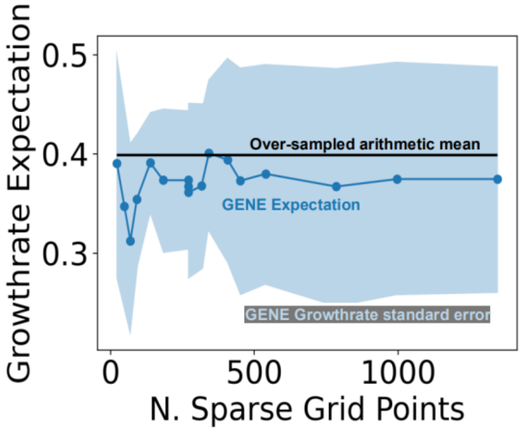


Fig 2: The surplus refined spatially adaptive sparse grid (blue), does not converge to the 'true' expectation (black). The shaded region shows the standard deviation from the expected value, defined as, $\sqrt{Var(f(\vec{x}))}$.

The surplus based strategy oversampled at the discontinuities, causing it to poorly generalise in the smooth regions (Fig 3). When the interpolator is tested against a pseudorandom test set, the number of outliers for static sparse grid of 25 samples is less than the adaptive sparse grid of 1346 where most of the samples have been placed at the discontinuities (Figs. 3a, b & c). The outliers are defined as having an error more than two standard deviations away from 0 error. When plotting the outliers on a histogram over the input space it is clear there are more outliers further from the discontinuity (Figs. 3d & e). The next step will be to try improving exploration over exploitation by including some volume based adaptive refinement cycles.

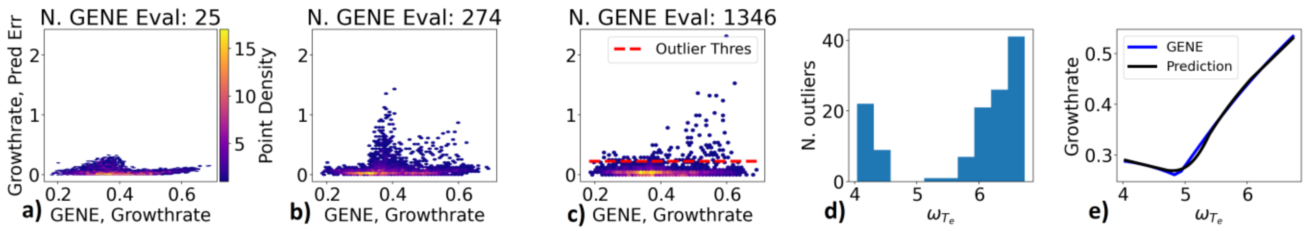


Fig 3 a,b,c: The difference between the interpolant and GENE (Pred Err) for a test set of 3000 samples. 25 point sparse grid and larger spatially adaptive grids. d,e: The outliers exist further from the discontinuities, $\omega_{T_e} = 4.9$.

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