Discretization Error Estimation and Mesh Optimization for Plasma Edge Transport Simulations of Nuclear Fusion Tokamaks

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Preface

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Abstract

In nuclear fusion, tokamak devices are the most advanced technology of magnetic confinement, in which the divertor configuration allows to control plasma-edge motion and power and particle exhaust. In this sense, computational simulations are an indispensable tool to study and characterize the plasma-edge physics. A key aspect is the selection of a suitable mesh that discretizes the spatial domain and allows to capture accurately the steep gradients of state variables and complex behavior of the plasma-edge.

In the first part of this work, different discretization error estimation methodologies are collected from the field of CFD to study their applicability to a plasma-edge model. It is found that Richardson extrapolation is the most suitable discretization error estimation strategy in terms of accuracy, computational cost and implementation cost. Richardson Extrapolation methodology is thus applied to the plasma-edge problem in order to estimate the distribution of discretization error of the ion density and ion temperature over the 2D simplified domain, so-called slab case. The mesh is defined by an exponential refinement toward the divertor targets. The analysis of the observed order of accuracy reveals that several regions present non-asymptotic behavior. In order to fix this problem, the discretization errors are converted into uncertainty errors by the GCI method. Results showed that the highest relative errors for the ion density are concentrated at the targets in the scrape-off layer. For the ion temperature, maximum relative errors are located near the X-point.

In the second stage of the thesis, the goal of finding a mesh adaptation method for reducing the discretization errors of the plasma state variables is tackled. First, it is concluded that the best error sensor candidates for guiding the adaptation process are feature-based error indicators and Richardson-based error indicators. An adaptation with two different approaches of the classical undivided difference detector to structured grids is proposed. After the application to the plasma-edge model, it is demonstrated that these feature error sensors do not provide sufficient accuracy for driving a mesh adaptation process to reduce the discretization errors.

The final contribution of this work is the development of a mesh optimization method aiming relative discretization error reduction applied to the plasma-edge model. A cost functional based on Richardson extrapolation as error adaptive sensor is presented. Two optimization strategies are tested: (i) the steepest descent method without line search and (ii) BFGS with line search satisfying Wolfe conditions. After an application test, a relative discretization error reduction from 15% to 5% is achieved between the maximum values of both configurations.
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Resumen ejecutivo

En la fusión nuclear, el tokamak es la tecnología más avanzada de confinamiento magnético, en el cual la configuración en divertor permite el control del movimiento del borde del plasma así como la extracción de potencia y la eliminación de partículas. En este sentido, las simulaciones computacionales constituyen una herramienta indispensable para estudiar y caracterizar la física del borde del plasma.

En la primera parte de este trabajo, se recogen las diferentes metodologías para estimar el error de discretización para estudiar su aplicabilidad al modelo del borde del plasma. Tras el análisis, se concluye que la Extrapolación de Richardson es la técnica más apropiada en cuanto a precisión, coste computacional y dificultad de implementación. Posteriormente, se aplica la Extrapolación de Richardson al modelo del borde del plasma para estimar la distribución de error de discretización de la densidad y temperatura iónicas en un dominio bidimensional simplificado. El mallado estudiado se caracteriza por un refinamiento exponencial hacia los platos del divertor. El análisis del orden de convergencia observado revela que ciertas zonas presentan comportamiento no asintótico con el refinamiento. Para solucionar dicho problema, los errores de discretización se convierten en estimadores de incertidumbre mediante el método GCI. Los resultados muestran que los errores relativos más elevados se concentran en los targets para la densidad iónica y cerca del punto magnético X, para la temperatura.

En la segunda fase del trabajo, el objetivo es encontrar un método adaptativo del mallado que reduzca los errores de discretización de las variables del plasma. Primero, se obtiene que los mejores candidatos de sensor del error para guiar el proceso adaptativo son indicadores basados en características del flujo e indicadores basados en la Extrapolación de Richardson.

Para ello, se propone una modificación para mallas estructuradas con dos posibles estrategias de aplicación para el detector de diferencias. Después de su aplicación al modelo del plasma, se demuestra que dichos indicadores no proporcionan suficiente precisión para guiar el proceso de adaptación de la malla.

La contribución final del trabajo es el desarrollo de un algoritmo adaptativo de optimización del mallado que reduce los errores relativos de discretización de las variables del plasma. Para ello, se diseña una función objetivo basada en los indicadores de Extrapolación de Richardson y se utilizan dos estrategias de optimización diferentes que permiten automatizar el proceso. Tras su aplicación, se consigue para un caso práctico una reducción muy importante del error relativo máximo, que desciende del 15% al 4.5%.
Resumen extendido

La fusión nuclear es una de las fuentes de energías más prometedoras para convertirse en una solución definitiva a las necesidades energéticas de nuestra sociedad en un futuro próximo. Es una energía limpia en la cual no se generan gases de efecto invernadero y su combustible puede considerarse como inagotable, pues el hidrógeno es el elemento más abundante en el universo. Su principio de funcionamiento está basado en la reacción nuclear en cual dos isótopos de hidrógenos son fusionados para formar helio. El defecto de masa que ocurre en dicho proceso se convierte en una gran liberación de energía de acuerdo con la ecuación de equivalencia masa-energía de Einstein $E = mc^2$.

Desarrollar una tecnología que reproduce los eventos que ocurren en el núcleo de una estrella es tal reto que será considerado como uno de los más grandes logros científicos de la historia de la humanidad. Para conseguir dicho fin, muchos problemas tienen que ser aún resueltos. El próximo paso para llegar a este objetivo podría ser ITER, un tokamak de 500 MW de potencia que está actualmente en fase de construcción en Francia, el cual pretende sentar las bases de las futuras centrales de fusión de escala comercial. En un tokamak, la combinación de bobinas y corriente inducida por un transformador central se utilizan para crear un fuerte campo magnético capaz de confinar y controlar el plasma. Mediante la introducción de un punto magnético X, la configuración en divertor permite controlar el movimiento del plasma en el borde y ayudar a la extracción de potencia y partículas mediante el direccionamiento del plasma que escapa de la última superficie cerrada de flujo magnético hacia los platos del divertor. En el borde del plasma tiene lugar una compleja combinación de fenómenos que incluye la interacción entre iones y electrones acelerados en un campo magnético y partículas neutras, que aparecen después de procesos de recombinación y son lanzadas hacia el plasma en un proceso de conocido como reciclaje. En este sentido, las simulaciones computacionales constituyen una herramienta indispensable para estudiar y caracterizar la física del borde del plasma.

Los códigos SOLPS (Scrape-Off Layer Plasma Simulation) son el resultado del acoplamiento entre un código multifluido como B2 y un código de Monte Carlo como Eirene, que simula las trayectorias de las partículas neutras [24]. Una de sus principales inconvenientes es el extremado coste computacional que se requiere para una simulación realista, que puede convertirse en inviable en ciertas aplicaciones. Debido a ello, la Division of Applied Mechanics and Energy Conversion de la universidad KU Leuven ha desarrollado en los últimos años una versión simplificada en Matlab, cuyo objetivo es conseguir un progreso más veloz en la investigación al
poder probar nuevas aplicaciones antes de ser implementadas en el código completo B2-Eirene.

En el corazón de estos códigos numéricos, se realiza la discretización de las ecuaciones diferenciales y el dominio mediante el método de volúmenes finitos. Esta fase juega un papel muy importante en la obtención de una solución numérica que aproxima con gran fidelidad la solución matemática exacta. Por tanto, un aspecto clave es la selección de la malla apropiada, alineada con las líneas de campo magnético, que discretiza el espacio físico y permite capturar con precisión los enormes gradientes de las variables de estado y el complejo comportamiento del plasma en el borde.

La estimación de los errores de discretización ha sido extensamente estudiada en las últimas décadas en un esfuerzo por mejorar las simulaciones numéricas de muchos problemas de ingeniería, resultando en diversas metodologías adaptadas a cada tipo de estrategia de discretización [29][22][26]. Muchas investigaciones se han concentrado en el campo de la fluidodinámica computacional [14] (y sus referencias), las cuales han servido recientemente como inspiración para aplicaciones de simulación del borde del plasma [25]. En la primera parte de este TFM, se estudian los diferentes métodos para la estimación de errores de discretización de las variables de estado del modelo del borde del plasma. Las técnicas más apropiadas serán aplicadas a un caso práctico con el objetivo de predecir la distribución de errores de discretización a lo largo del dominio, incluyendo un estudio de los factores que más influyen en la fiabilidad de los estimadores.

En la segunda parte, se analizará la posible aplicación de estrategias adaptativas de mallado al modelo del borde del plasma. Varios ejemplos de refinamiento adaptativo en el borde plasmático se pueden encontrar en [4][19]. Métodos muy innovadores basados en optimización con ecuaciones diferenciales en derivadas parcial como restricciones (PDE-constrained optimization) se han aplicado para automatizar el diseño del campo magnético de divertores [3][7]. Este trabajo pretende extender esta metodología para el diseño adaptativo de mallas para obtener configuraciones óptimas que minimizan los errores de discretización de las variables del modelo del borde del plasma.

Por tanto, el objetivo de este trabajo es doble: Primero, estudiar los métodos de estimación más apropiados del error de discretización para posteriormente evaluar la precisión numérica de las configuraciones de malla típicas de un tokamak con configuración de divertor. Y segundo, la búsqueda de un método adaptativo de mallado para la obtención de configuraciones de malla óptimas adaptadas a una solución, en consecuencia mejorando la precisión numérica con un coste de computación aceptable. Las técnicas desarrolladas en este trabajo podrían ser aplicadas a un código de simulación completo de borde de plasmas como B2-Eirene.

**El modelo del plasma**

El modelo en Matlab de borde del plasma se deriva de modelos de B2-Eirene utilizando algunas simplificaciones que garantizan suficiente precisión para describir con fidelidad los procesos físicos. B2 emplea la hipótesis de alta colisionalidad para describir el
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transporte de partículas cargadas con un modelo multi-fluido. Por otro lado, el transporte de partículas neutras es tratado de forma cinética por Eirene, aumentando severamente el coste computacional. Para reducir éste, la primera simplificación es la sustitución de la simulación de Monte Carlo por un modelo fluido para el transporte de neutrales. Adicionalmente, el modelo se convierte en un problema bidimensional en el plano poloidal gracias a la simetría en la dirección toroidal. Finalmente, el dominio es simplificado a uno de tipo rectangular con cortes, denominado slab case (caso loseta).

La gran anisotropía en el transporte obliga a la discretización a usar mallas alineadas con las líneas de campo manético, para poder separar el transporte radial y poloidal evitando la contaminación numérica del transporte radial por errores de aproximación. En dicha topología con celdas rectangulares, dos caras se encuentran alineadas con el campo magnético mientras que las otras son perpendiculares al mismo en la dirección radial. Las condiciones de contorno incluyen velocidad isotermica sónica en los platos del divertor, potencia y densidad fija en la frontera del núcleo así como flujo de neutrales nulo en dicha región. Además, se especifican condiciones de recirculación de los neutrales en la capa externa. El sistema de ecuaciones se expresa en sistema de coordenadas poloidal-radial. Dichas ecuaciones se resumen en la ecuación de continuidad del plasma, la ecuación de conservación de la cantidad de movimiento en dirección paralela al campo magnético, la ecuación de conservación de la energía y la ecuación de difusión de los neutrales. Debido a que dichas ecuaciones se pueden escribir como un conjunto acoplado de ecuaciones de tipo convección-difusión, la discretización empleada es el método de volúmenes finitos. Los esquemas de discretización para aproximar los flujos son una combinación de esquemas upwind, lineales e híbridos. Finalmente, el sistema no lineal de ecuaciones se resuelve mediante un método iterativo.
Estimación del error de discretización

El error de discretización $\varepsilon_h$ se define como la diferencia entre la solución exacta del modelo matemático y la solución del sistema algebraico de ecuaciones obtenido de la discretización, como muestra la expresión:

$$\varepsilon_h = u_h - u.$$  \hspace{1cm} (1)

Dicho error depende principalmente del esquema de discretización empleado, de la calidad de la malla, y del comportamiento de la solución y sus derivadas. De entre los tipos de errores numéricos, es el que presenta mayor dificultad para estimar así como el de mayor coste computacional, ya que normalmente requiere múltiples soluciones en diferentes niveles de mallado [29]. Además, suele representar la fuente de mayor error de tipo numérico. A continuación se presenta de forma muy resumida las principales metodologías de estimación del error de discretización, recogidas del campo de la fluido dinámica computacional para estudiar su posible aplicabilidad al modelo del borde de plasma. El objetivo es encontrar la técnica de estimación más apropriada para el modelo del plasma. Los principales puntos para la comparación son la precisión, el coste computacional y la dificultad de implementación.

Métodos de mayor orden de convergencia

Dichos métodos comparan la solución discreta a una estimación de la solución matemática del modelo de mayor orden. Normalmente requieren de múltiples soluciones en diferentes mallas sucesivamente refinadas entre sí o de diferente orden de convergencia.

1. **Refinamiento de malla: Extrapolación de Richardson** La Extrapolación de Richardson emplea tres mallas con un factor de refinamiento entre ellas para obtener una solución extrapolada de orden $p + 1$. Dicha solución se utiliza después para estimar el error de discretización y en caso de que se muy fiable, puede ser incluso utilizada para corregir la solución de la malla más fina. El estimador de la solución matemática se obtiene de la expresión:

$$\bar{u} = u_h + \frac{u_h - u_{r+h}}{r^p - 1},$$  \hspace{1cm} (2)

Con $p$ el orden de convergencia del esquema de discretización y $r = \frac{h_{coarse}}{h_{fine}}$. De la solución extrapolada $\bar{u}$, se obtiene el estimador del error de discretización:

$$\varepsilon_h = u_h - \bar{u} = -\frac{u_h - u_{r+h}}{r^p - 1}. $$  \hspace{1cm} (3)

2. **Métodos de refinamiento de** $p$ Estas técnicas emplean dos o más discretizaciones en la misma malla pero con diferente orden formal de convergencia. Posteriormente, combinan dichas soluciones para estimar el error de discretización. Un ejemplo representativo es el método de Kutta-Feuhberg [10].
Métodos basados en el residuo

El cálculo del estimador del error de discretización se basa en el error de truncación, conocido como residuo. Existen dos tipos principales:

1. **Ecuaciones de Transporte del Error de Discretización (DETE, en inglés)** El error de discretización se transporta a lo largo del dominio de forma similar a la solución:

   \[ L_h(\varepsilon_h) = -TE_h, \tag{4} \]

   Existen a su vez dos posibilidades: el método continuo y el método discreto. Normalmente, el error de truncación que es el término fuente del sistema de ecuaciones es aproximado mediante otras estrategias.

2. **Metodología Adjoint** Esta técnica se utiliza para estimar errores de discretización de variables globales \( f(u) \), como puede ser la carga térmica total en los platos del divertor.

   \[ \varepsilon_h = f_h(u_h) - f_h(u). \tag{5} \]

   Después, mediante el empleo de series de Taylor se obtiene la siguiente ecuación (método Adjoint discreto):

   \[ f_h(u) = f_h(u_h) + \left. \frac{\partial f_h}{\partial u} \right|_{u_h} \cdot \left( \left. \frac{\partial L_h}{\partial u} \right|_{u_h} \right)^{-1} \cdot L_h(u). \tag{6} \]

   En el cual el vector de soluciones adjoint es \( \psi_T \), que representan las sensibilidades de la solución con respecto a las fuentes locales de error.

El análisis comparativo de cada una de las metodologías explicadas anteriormente se puede resumir en las siguientes conclusiones:

1. En principio, los métodos de mayor orden de convergencia obtienen estimadores de mayor precisión mientras que los métodos residuales consiguen también alta precisión dependiendo de la calidad de estimación del error de truncación.

2. La metodología DETE proporciona el menor coste computacional en la teoría. Sin embargo, si se desea alta precisión en la estimación del error de truncación, se requiere de simulaciones adicionales de forma que iguala finalmente el coste de métodos Adjoint o de mayor orden de convergencia.

3. El coste de implementación es por tanto el factor diferencial que determina la elección de un método particular. En este sentido, la Extrapolación de Richardson presenta la menor dificultad en comparación con otros métodos intrusivos del código, como DETE y refinamiento del orden, o comprado con aquellos que requieren del complejo cálculo de Jacobianos, como la metodología Adjoint.
Resumen extendido

En cada uno de los métodos explicados, se requiere una estimación basada en soluciones más refinadas ya sea a través de la estimación del error de truncación (métodos residuales) o por la propia metodología (métodos de mayor orden de convergencia). Por tanto, es obligatorio un estudio sobre la fiabilidad de los estimadores basado en el comportamiento de la solución cuando es refinada. Dicho comportamiento se obtiene mediante el cálculo del orden de convergencia del error de discretización. Para que un estimador se considere como fiable, el orden de convergencia calculado debe ser igual al orden formal de los esquemas de discretización empleados. Para que se cumpla dicha condición, existen cinco requisitos fundamentales: (i) las soluciones refinadas deben encontrarse en la región asintótica, (ii) el mallado debe ser Cartesiano o al menos deben emplearse mallas con suficiente regularidad, (iii) las mallas empleadas deben estar relacionadas por refinamiento sistemático, (iv) las soluciones deben ser diferenciables y (v) las otras fuentes de error numéricos deben ser pequeñas.

Este paso es la razón fundamental para escoger la Extrapolación de Richardson: para el test de fiabilidad es esencial el cálculo del orden de convergencia para comprobar aquellas regiones donde no coincide con el orden formal. Por tanto, tres mallas sistemáticamente refinadas son necesarias para este proceso, el cual constituye un paso intrínseco en la Extrapolación de Richardson. En conclusión, La Extrapolación de Richardson es el método de estimación del error de discretización más apropiado para el modelo del borde del plasma estudiado en este trabajo.

Implementación de la Extrapolación de Richardson al modelo del plasma

En este capítulo, se aplica la Extrapolación de Richardson al modelo del borde del plasma con el objetivo de estimar la distribución del error de discretización de la densidad iónica y de la temperatura iónica. El dominio se discretiza con dos tipos de mallas: (i) la denominada malla biased con 280x80 celdas, que se caracteriza por un refinamiento exponencial hacia los targets del divertor y (ii) la malla bezier con 720x40 celdas, que comprende dos zonas con diferentes niveles de refinamiento poloidal equidistantes unidas por una transición suave definida por una curva de bezier.

El método empleado en el algoritmo para reconstruir las soluciones en los nodos de la malla gruesa es un procedimiento de integración, que cumple la condición de utilizar esquemas de mayor orden de convergencia que el orden formal para evitar la introducción de otros errores.

El análisis del orden de convergencia de los errores de discretización para cada variable en caso de la malla biased revela varias regiones del dominio con convergencia muy lenta o incluso comportamiento no asintótico. Por tanto, dichas zonas presentan baja fiabilidad en la estimación de errores. La principal sospecha sobre este tipo de comportamiento es la baja calidad de la malla, la cual presenta transiciones muy bruscas en el refinamiento de las celdas debido al refinamiento exponencial. Por este motivo, se emplea la malla bezier, caracterizada por una buena calidad de malla por ser muy uniforme, con el objetivo de verificar la hipótesis de que la calidad del
mallado es la responsable del deterioro en el orden de convergencia. El resultados demuestran una mejora muy significativa del orden de convergencia para esta malla uniforme. Sin embargo, ciertas regiones del dominio aún presentan comportamiento no asintótico, que podría ser explicado por refinamiento insuficiente o incluso podrían ser causado por características locales del problema, como el caso de comportamiento oscilatorio que ocurre cuando se combina esquema de discretización con órdenes de convergencia mixtos en ecuaciones de tipo convección-difusión [6].

**Figure 2:** Distribución del orden de convergencia de la densidad iónica sobre el dominio bidimensional para la malla biased de 280x80 celdas.

**Figure 3:** Distribución del orden de convergencia de la temperatura iónica sobre el dominio bidimensional para la malla biased de 280x80 celdas.

Para resolver el problema de fiabilidad asociado a las regiones de convergencia lenta o comportamiento no asintótico, los errores de discretización se convierten en estimadores de incertidumbre mediante el método Grid Convergence Index con las recomendaciones de Oberkampf and Roy [22]. Esta técnica permite mejorar la confianza mediante el cálculo de estimadores del error de discretización con un 95% de probabilidad de que el verdadero error se encuentre dentro de una banda de error de incertidumbre. Después de su aplicación a los dos tipos de mallados estudiados
anteriormente, se obtiene finalmente la distribución de error de discretización para cada una de las variables del plasma en cada caso.

En cuanto a la densidad de iones de malla biased, los errores de discretización más elevados se concentran en los targets del divertor, proporcionando valores alrededor del 5%. Esto se debe a la dificultad de capturar con detalle los enormes gradientes en dicha región, incluso para una malla con refinamiento exponencial, además del comportamiento no asintótico de dicha región. La región privada del plasma también presenta errores entre 3% and 4%, mientras que la zona central obtiene errores muy bajos. Respecto a la temperatura iónica, los errores relativos máximos (8.7% - 10.4%) se encuentran cerca del punto magnético X. Además, en la SOL (Scrape-Off Layer) aparecen errores del 6.5% que se extienden a lo largo de la separatrix.

**Figure 4:** Distribución del error de discretización (%) de la densidad iónica en perspectivas 3D y 2D para la malla biased de 280x80 celdas.

Por otro lado, los resultados de la malla bezier muestran una distribución de error muy similar pero con magnitudes inadmisibles (hasta el 40% para la densidad iónica y 25% para la temperatura iónica), conformando que la mejora en el orden
Resumen extendido

Figure 5: Distribución del error de discretización (%) de la temperatura iónica en perspectivas 3D y 2D para la malla biased de 280x80 celdas.

de convergencia no justifica la selección de este tipo de malla uniforme debido a su pobre resolución para el borde del plasma.

Finalmente, se puede concluir que la malla de tipo biased (refinamiento exponencial) es una solución adecuada para capturar la naturaleza extrema del borde del plasma obteniendo errores de discretización admisibles en comparación con otras mallas más uniformes.

Adaptación del mallado para reducir el error de discretización

En la segunda parte de este trabajo, se centra en el objetivo de encontrar un método de mallado adaptativo para reducir el error de discretización de las variables del borde del plasma. El primer paso es por tanto la búsqueda de un sensor del error
Resumen extendido

adecuado para este propósito, denominado normalmente como indicador del error.

Con la premisa de no cambiar la estructura de datos interna del código, se escogen los métodos que redistribuyen los nodos de la malla (r-refinement) o que dividen las celdas (h-refinement) como las estrategias posibles para mejorar la precisión de las simulaciones numéricas.

Los mejores candidatos de sensor del error para guiar el proceso adaptativo son indicadores basados en características del flujo (feature-based error indicators) e indicadores basados en la Extrapolación de Richardson. La principal ventaja del detector de diferencias es el bajo coste computacional ya que sólo requiere de una única simulación. Este tipo de sensores funciona correctamente capturando fenómenos característicos del flujo (e.g. fuertes gradientes), aunque carece de base matemática al no estar directamente relacionados con los errores de discretización.

La posible aplicabilidad al modelo del plasma debe ser comprobada. Por otro lado, los indicadores basados en la Extrapolación de Richardson permiten calcular los verdaderos errores de discretización evitando posibles problemas de convergencia asociados con métodos de estimación del error de truncación (e.g. τ-estimation) o el prohibitivo coste de implementación de métodos que requieren la obtención de Jacobianos del sistema. Sin embargo, el coste computacional es mayor ya que requieren de varias soluciones. Por tanto, los sensores basados en la Extrapolación de Richardson junto a una estrategia de optimización se convierten en el segundo candidato para el método adaptativo de la malla.

Implementación del detector de diferencias al modelo del plasma

En este capítulo, los indicadores basados en características del flujo se implementan en el modelo del plasma con el objetivo de comprobar la precisión de estos sensores del error para poder guiar un posible método de refinamiento (h-refinement). El detector de diferencias se define como la diferencia entre la solución en una celda y la solución de las celdas colindantes. Este parámetro permite almacenar el cambio en la solución de una celda a la siguiente, proporcionando información sobre cómo la malla captura la solución en cada dirección. La implementación de se realiza ala densidad y temperatura iónicas en una malla de 70x20 celdas con refinamiento exponencial (biased grid).

La estrategia clásica de dividir celda a celda utilizando estos indicadores se ha realizado anteriormente en [19]. Esta técnica generalmente solo es posible aplicarse en mallas sin estructura, en la que los nodos que quedan sueltos no resultan ser un problema para su almacenamiento. Sin embargo, el código en Matlab empleado en este trabajo utiliza una estructura de datos que no permite nodos colgantes. Por tanto, se proponen otras estrategias que respetan la estructura actual de datos. Un simple procedimiento consiste en dividir columnas o filas enteras en vez de celdas únicas. Hay dos posibles estrategias en este sentido. La primera consiste en calcular la media de los indicadores a lo largo de cada dirección, mientras que la segunda emplea el máximo valor de cada columna o fila. Estos indicadores se comparan con...
Resumen extendido

unos límites establecidos para decidir si se divide o se ensancha dicha columna o fila en cuestión. En la figura se muestra un ejemplo de indicador poloidal para la temperatura iónica, obtenido con la técnica del indicador máximo.

![Figure 6](image)

**Figure 6:** Indicador poloidal máximo Cy de la temperatura iónica antes y después de ser seleccionado para su refinamiento.

Con el objetivo de comprobar la precisión de estas estrategias, se comparan con los perfiles del error de discretización obtenido con la Extrapolación de Richardson. Los resultados muestran que únicamente para ciertos casos los indicadores capturan con precisión las regiones de mayor error de discretización, mientras que para otro casos los mismo indicadores no localizan dichas regiones. Por tanto, la precisión de los indicadores depende de cada caso particular y no pueden ser generalizados para cualquier aplicaciones. Un ejemplo de estos resultados se proporciona en la figura, en la cual el indicador poloidal máximo consigue alta precisión para la temperatura iónica (figura superior) pero fracasa totalmente para la densidad iónica (figura inferior).

Por tanto, se concluye que el detector de diferencias no proporciona precisión suficiente para guiar un algoritmo adaptativo para el modelo de borde del plasma estudiado en este trabajo.
Resumen extendido

Figura 7: Comparación del indicador poloidal máximo Cy con el error de Richardson para el caso de la temperatura iónica (figura superior) y densidad iónica (figura inferior).

Optimización del mallado utilizando la Extrapolación de Richardson como sensor del error

Este capítulo final estudia la aplicación de métodos de optimización con ecuaciones diferenciales como restricciones (PDE-constrained optimization) al modelo del plasma con el objetivo de reducir el error de discretización de una variable deseada. El sensor del error que ayuda a construir la función objetivo se obtiene por la Extrapolación de Richardson. En los métodos de optimización con ecuaciones diferenciales como restricciones, las variables de estado pueden ser eliminadas del problema resultando en una problema de optimización reducido, en el cual los parámetros de malla son las únicas variables de control. El caso de aplicación tiene como objetivo encontrar una malla con un parámetro óptimo de malla que minimiza el error relativo de discretización de una variable de estado, en este caso, la densidad iónica. Por tanto, la configuración de malla a ser optimizada es conocida como biased grid por zonas, que consiste en una malla dividida en tres regiones separadas por los cortes en cada cual existe un refinamiento poloidal exponencial hacia los bordes, definido por un único parámetro de control denominado biased factor.

Con el objetivo de reducir el error relativo en los targets, es importante que los errores calculados después de cada iteración sean comparados en los mismos puntos
físicos, ya que los nodos se desplazan por el dominio con cada actualización de la variable de control. Para ello, se introduce un paso intermedio que interpola los errores de malla actual a una malla equidistante que se mantiene constante en todo el proceso. La solución de referencia que proporciona el sensor del error de discretización para guiar el proceso se obtiene de la Extrapolación de Richardson utilizando dos mallados en cada iteración (el mallado de la iteración actual y un mallado más grueso auxiliar), asumiendo el orden de convergencia como constante. Esta opción proporciona una función objetivo que estima con suficiente precisión el error de discretización con un coste computacional aceptable. El algoritmo usa un método de tipo Newton para resolver el problema de optimización, en el que se emplean dos estrategias diferentes para aproximar el Hessiano de la función objetivo: (i) el método Steepest descent y (ii) el método BFGS satisfaciendo condiciones de Wolfe. Los gradientes respecto a la variable de control se calculan mediante diferencias finitas en cada iteración. Antes de la implementación, se reliza un mapeado de la función objetivo para el caso particular estudiado, para poder confirmar si el algoritmo alcanza el verdadero mínimo global, localizado en \( b = 0.825 \) y se comprueba que no es necesario el uso de soluciones completamente convergidas para obtener dicha función.

Tras la optimización, se obtiene que la variable de control evoluciona de un punto inicial \( b_0 = 0.95 \) hasta converger al valor óptimo \( b_{opt} = 0.8257 \). Respecto al método Steepest descent, el algoritmo ha necesitado 17 iteraciones mientras que el método BFGS mejora su rendimiento necesitando únicamente 5 iteraciones. Esta última estrategia es en general la más apropiada cuando uno desea optimizar casos de mayor complejidad, en los cuales no se tiene información previa de la función objetivo y por tanto use requiere de un método más automatizado.

El algoritmo de optimización ha obtenido por tanto una configuración de malla que minimiza error de discretización. Para verificar dicha reducción, se representan los errores relativos de discretización de la densidad iónica para la malla inicial y final, en el cual se observa que se ha conseguido una reducción muy importante del error relativo máximo, que desciende del 15% al 4.5% (figura 9).
Conclusiones generales

Finalmente, se pueden resaltar las siguientes conclusiones generales:

1. La Extrapolación de Richardson es el método más apropiado de estimación de error de discretización para el modelo de borde del plasma.

2. La aplicación de la Extrapolación de Richardson al modelo del plasma con una mallado de tipo exponencial muestra que los máximos errores relativos se encuentran en los targets para la densidad iónica y cerca del punto magnético X para la temperatura iónica.

3. La malla de tipo biased (refinamiento exponencial) es una solución adecuada para capturar la naturaleza extrema del borde del plasma obteniendo errores de discretización admisibles en comparación con otras mallas más uniformes.

4. El detector de diferencias no proporciona precisión suficiente para guiar un algoritmo adaptativo para el modelo de borde del plasma estudiado en este trabajo.
5. Se ha desarrollado un algoritmo adaptativo del mallado basado sensores del error obtenidos con la Extrapolación de Richardson, que permite la obtención de configuraciones malla óptimas que reducen el error relativo de discretización de las variables del plasma elegidas.

**Figura 9:** Reducción del error relativo de discretización conseguido en la optimización.
List of Abbreviations and Symbols

Abbreviations

AMR Adaptive Mesh Refinement
CFD Computational Fluid Dynamics
CPU Central Processing Unit
DE Discretization Error
DETE Discrete Error Transport Equations
FV Finite Volumes
GCI Grid Convergence Index
GHG Green House Gas
PDE Partial Differential Equation
PF Private Flux
RE Richardson Extrapolation
SOL Scrape-Off Layer
SOLPS Scrape-Off Layer Plasma Simulations
TE Truncation Error

Symbols

c Speed of light
E Energy
m Mass
∥ Parallel curvilinear coordinate
⊥ Diamagnetic curvilinear coordinate
r Radial curvilinear coordinate
θ Poloidal curvilinear coordinate
ϕ Toroidal curvilinear coordinate
n Particle density
V Particle velocity
S Source term
Zi Charged state of ions
u∥ Parallel velocity
ur Radial velocity
\eta \quad \text{Viscosity tensor}
\nD \quad \text{Diffusion coefficient}
\n\rho \quad \text{Pressure}
\nt \quad \text{time}
\nT \quad \text{Temperature}
\n\Gamma \quad \text{Particle flux}
\n\kappa \quad \text{Heat conductivity tensor}
\nT \quad \text{Temperature}
\n\varepsilon_h \quad \text{Discretization error}
\nTE_h \quad \text{Truncation error}
\n\hat{p} \quad \text{Observed order of accuracy}
\nx \quad \text{Poloidal direction}
\ny \quad \text{Radial direction}
\nJ \quad \text{Jacobian}
\nU_h \quad \text{Discrete forward solution}
\nC \quad \text{difference detector}
\n\Psi \quad \text{Adjoint solution}
Chapter 1

Introduction

Nuclear fusion is one of the most promising energy sources to become a definitive solution to our society’s energy needs in the near future. It is a clean energy in which no GHG emissions are generated and its fuel can be considered inexhaustible, as the hydrogen is most abundant element in the universe. The working principle is based on the nuclear reaction in which two isotopes of hydrogen are fused to form helium. The mass defect that occurs in this process is transformed into a great release of energy following the Einstein’s equation of mass-energy equivalence \( E = mc^2 \).

Developing a device that reproduces the events that happen inside of the core of a star is such a challenge that it will be considered one of the greatest technological achievements of human history. To this end, many important issues are still to be solved. The next step to reach this goal may be ITER, a tokamak device of 500 MW currently under construction in France, which aims to provide the basis for future industrial-scale power plants. In a tokamak, coils along with an induced current by a central transformer are used to create a strong magnetic field that confines and controls the plasma. By the introduction of an magnetic X-point, the divertor configuration allows to control the plasma-edge motion and help power exhaust and particle removal by directing the plasma that passes through the last closed magnetic flux surface toward the divertor targets. A complex combination of phenomena occurs in the plasma-edge that involves interaction between ions and electrons, that are accelerated in the magnetic field, and neutral particles that appear after recombination and are projected back into the plasma in a process called recycling. In this sense, computational simulations are an indispensable and powerful tool to study and characterize the plasma-edge physics.

SOLPS (Scrape-Off Layer Plasma Simulation) codes are built from the multi-fluid code B2 coupled to Monte Carlo code Eirene, which simulates the trajectories of neutral particles [24]. One of the biggest constrains of these codes, developed by international cooperation, is the extremely computational cost required for a realistic simulation, that at some applications can even become unfeasible. In this sense, the Division of Applied Mechanics and Energy Conversion of KU Leuven has developed in the recent years a simplified version of the full code in Matlab, which aims to make a faster progress in research by testing applications before implementing them into
B2-Eirene. Inside these numerical codes, a discretization of the partial differential equations and domain by finite volumes is performed. This stage plays a very important role on obtaining a solution that approximates with high fidelity the real exact solution. Therefore, a key aspect is the selection of a suitable mesh aligned with the magnetic field lines that discretizes the spatial domain and allows to capture with detail the steep gradients of state variables and complex behavior of the plasma-edge.

The estimation of discretization errors has been extensively studied in the last decades in an effort to improve the numerical simulations of many engineering problems, resulting in diverse methodologies adapted to each type of discretization strategy [29][22][26]. Many research has been focused on the field of computational fluid dynamics [14] (and references therein), which has served recently as inspiration for plasma-edge applications [25]. In the first stage of this work, the different methodologies for estimating the discretization error of the state variables of a plasma-edge model are discussed. The most suitable technique will be applied to a practical case in order to predict the discretization error distribution over the domain including a study of the most important factors that influence the reliability of these estimates. In the second stage, the possible application of mesh adaptive strategies to the plasma-edge model will be analyzed. Several examples of adaptive refinement on scrape-off layer plasmas can be found in literature [4] [19]. Innovative methods based on PDE-constrained optimization have been applied to automatize magnetic divertor design in [3][7]. This work aims to extend this approach to mesh design in order to obtain optimal configurations that minimize the discretization errors of plasma-edge variables.

Therefore, the motivation for this work is twofold: First, to study suitable discretization error estimates to evaluate the numerical accuracy of typical grids used in a tokamak divertor configuration; and second, the search of a mesh adaptive methodology to obtain optimal grid configurations adapted to a solution, thereby improving the numerical accuracy with a good compromise of computational cost. The techniques developed in this work would be able to be extended to full plasma-edge codes such as B2-Eirene.

The thesis outline has the following structure: Chapter 2 introduces the main aspects of the Matlab plasma-edge model. Chapter 3 collects the discretization error estimation methodologies and its applicability to a plasma-edge model. The implementation of Richardson extrapolation into a practical case is presented in Chapter 4, which aims to predict discretization error distribution of state variables and study the reliability of the estimates depending on grid factors. Chapter 5 starts the second stage by analyzing the different mesh adaptive strategies available from CFD along with error adaptive sensors. The best candidates for guiding the adaptation algorithm of the plasma-edge case are proposed. Chapter 6 explores the structured approach of feature-based error indicators and their application to the plasma-edge problem. Finally, a design optimization algorithm which allows to adapt the mesh to a state solution and thus minimize the relative discretization error is explained in Chapter 7. The general conclusions close the thesis.
Chapter 2

The plasma-edge model

In this chapter, the plasma edge model used for the thesis is presented. The completely
detailed derivation of the model is explained by Dekeyser in [7]. All its essential
points are collected here to provide a short overview. First, the simplifications used
in the Matlab code are described, followed by the coordinate system, geometry and
domain. Finally, the plasma-edge equations, finite volume discretization and solver
algorithm are introduced.

2.1 Main assumptions

With the goal of reducing the computational time to make faster progress in research
applications, the Matlab plasma-edge model is derived from B2-Eirene models using
some simplifications that still provide sufficient accuracy to describe with fidelity the
real physical processes. B2-Eirene code package is the result of a coupling between
the multifluid plasma-edge code B2 and Monte Carlo code Eirene [24]. B2 uses the
assumption of high collisionality to be able to use a fluid model to describe charged
particles motion in the scrape-off layer. On the other hand, recycling processes and
transport of neutral particles is treated kinetically by Eirene, with the expense of
high computational cost.

In order to save significant CPU time, the first assumption made for the simplified
model is the replacement of the Monte Carlo simulation by a neutral fluid transport
model. Additionally, deuterium is considered as the only ion species so that electron
density is derived from charge neutrality. The geometry corresponds to a regular
divertor configuration with one magnetic x-point. Due to toroidal symmetry, the
model becomes a 2D problem in the poloidal plane, which is simplified by an
isoparametric transformation into a rectangular domain, as it will be explained in
section 2.2.

2.2 Geometry and discretization of the domain

In a tokamak reactor, the magnetic field is created by the superposition of toroidal
and poloidal magnetic fields created by external coils and induced current respectively.
Two curvilinear coordinate systems are generally used in tokamak transport codes: (i) a parallel-diamagnetic-radial ($|\parallel, \perp, r$) coordinate system and (ii) a poloidal-radial-toroidal ($\theta, r, \phi$) coordinate system. The first one is suitable to describe the anisotropy in transport parallel and perpendicular to the magnetic field lines, whereas the second is very useful to take advantage of the toroidal symmetry, which allows to ignore the toroidal direction resulting in a 2D problem in the poloidal plane.

The 2D domain in the poloidal plane starts from a flux surface in the core region and extends radially covering the scrape-off layer (SOL) and private flux region (PF). In order to simplify the simulation, the physical domain is mapped to a rectangular domain, so-called the slab case. Please note the difference between the mapping that projects the computational grid on a rectangular domain to apply structured grid methods on the one hand and a slab case on the other hand. In the former, metric coefficients account for this transformation in the equations and as such no simplification is made. A "slab case" on the other hand, simplifies the geometry of the domain to such a rectangular domain, without including any metric coefficients that come along with the transformation. The great anisotropy in transport forces the spatial discretization to use again field-aligned grids to separate both processes and avoid numerical contamination of radial transport due to approximation errors. In this topology with quadrilateral cells, two faces are aligned with the magnetic field lines and the other are perpendicular to it, aligned with the radial coordinate direction. The transformation to the rectangular domain with cuts and its spatial discretization is shown is figure 2.2.
2.3 State plasma-edge equations

In this section, the general plasma-edge system of equations used in the model is presented. Then, the discretization of the PDE and numerical solver is discussed.

Plasma continuity equation

As charge neutrality is assumed, ion and electron densities are related through the expression \( n_e = Z_i n_i \), with \( Z_i \) the ions charged state. The plasma continuity equation is of the form

\[
\frac{\partial n_i}{\partial t} + \nabla \cdot (n_i \mathbf{v}_i) = S_{n_i},
\] (2.1)

where \( \mathbf{v}_i \) is the ion velocity and \( S_{n_i} \) is the source term involving ionization and recombination processes.

Parallel momentum equation

The tensorial momentum equation is projected onto the parallel coordinate direction yielding the sum of the ion and electron parallel momentum equations

\[
\frac{\partial}{\partial t} \left( m_i n_i u_{||} \right) + \nabla \cdot \left( m_i n_i u_{||} \mathbf{v}_i - \eta^i \nabla u_{||} \right) = S_{m_i u_{||}} - \nabla_{||} p,
\] (2.2)

where \( u_{||} \) is the ion and electron parallel velocity, \( p \) is the plasma pressure, \( \eta^i \) is the ion viscosity tensor and \( S_{m_i u_{||}} \) refers to the source term of momentum due to ionization and recombination. Electron inertia and viscosity are neglected. On the other hand, radial transport equation is not solved but replaced by a empirical anomalous diffusion equation of the form \( n_i u_r = -D^i \nabla_r n_i \) and the diamagnetic component is neglected as drifts are not considered.
2. The plasma-edge model

Neutral pressure diffusion equation

The neutral model is derived from neutral continuity equation and Navier-Stokes momentum equation, which is simplified by only retaining terms in the parallel direction, yielding a modified neutral pressure diffusion equation

\[
\frac{\partial n_n}{\partial t} + \nabla \cdot \left( n_{n,eq} u_{||} - D^n_p \nabla p_n \right) = S_{n_n},
\]

where \( n_n \) refers to neutral density, \( n_{n,eq} \) is a weighted neutral density, \( D^n_p \) is an isotropic diffusion coefficient and \( p_n \) is the neutral pressure.

Energy equation

Finally, the energy equation is obtained as the sum of the total energies for all species denoted by \( a \)

\[
\frac{\partial}{\partial t} \left( \frac{3}{2} \sum a n_a T \right) + \nabla \cdot \left( \frac{5}{2} \sum a \Gamma^a T - \kappa \nabla T \right) = S_E + \nabla u_{||} \cdot \eta^i \cdot \nabla u_{||} + u_{||} \nabla || p + V_n \cdot \nabla p_n,
\]

where \( T \) is the temperature for ions, electrons and neutrals. \( \Gamma^a \) refers to the particle flux of specie \( a \) and \( \kappa \) is the heat conductivity tensor.

Discretization and numerical solver

The main boundary conditions include sheath conditions at the targets in which the ions are assumed to reach isothermal plasma sound speed, fixed power and density at the core boundaries as well as no neutral flux to the core. In the outer wall, recycling conditions for the neutral are specified.

This system of equations is then expressed in the poloidal-radial coordinate system, which is more suitable for the numerical simulations. As they can be written as a set of coupled convection-diffusion equations, a finite volume discretization on the slab case domain with staggered grid configuration is performed. The discretization schemes to approximate fluxes are a combination of upwind, linear and hybrid schemes. Upwind schemes are used for the ion and neutral continuity equations. For energy and momentum equations, hybrid and linear schemes are employed.

Finally an iterative procedure to solve the non-linear discretized equations is applied which updates a plasma state variable after solving a correction equation. A pressure-correction equation is used to enforce ion continuity.
Chapter 3

Discretization error estimation

This chapter introduces the concept of discretization error and provides a literature review of the most important discretization error estimation methodologies. Then, the reliability of these estimates is discussed. Finally, the comparison of these techniques and its applicability to the plasma-edge problem is performed resulting in a selection of the most suitable one.

3.1 Application of a numerical simulation code

In any engineering problem, a mathematical model is required to express physical reality and it is always derived with an introduction of some sort of approximation.

In most engineering applications, such as fluid mechanics, heat transfer, electromagnetism or structural mechanics, and as seen in previous chapter, our particular case of plasma physics, a system of partial differential equations along with the associated initial and boundary conditions is used for describing the mathematical model. The most realistic models may depend on several spatial coordinates and time, local properties as well as include non-linearities... This complexity can lead to a model that is hard to solve analytically or analytical solutions might even not exist. Consequently, the use of numerical techniques to obtain approximations of the solutions provides a very powerful tool to solve these engineering problems [20]. Therefore, the scientific computing community has put great effort in developing numerical codes to provide solutions to all areas of engineering.

The creation and application of a simulation code is divided in four stages:

1. Modelling, which consists of comprehending physical reality and translating it into an appropriate mathematical model (e.g. a set of partial differential equations (PDEs)).

2. Discretization of both the partial differential equations and the domain, yielding a system of algebraic equations (or ordinary differential equations) and a set of discrete points in the domain in which the numerical solution will be obtained.

3. Solving the discretized system.
3. Discretization error estimation

4. Interpretation of results.

Every step in this process (except for step 4) can introduce error into the results respectively: (i) modelling errors, (ii) discretization and truncation errors and (iii) errors due to not exactly solving the discretized system (e.g. a remaining convergence error).

Modelling errors are defined as the difference between physical reality and the exact solution of the mathematical model. This type of errors are considered the most difficult to identify since one requires to perform rigorous experiments to obtain real data, which may not always be available, to be able to validate the model. In addition, modelling errors not only come from the lack of knowledge of reality, but also the process of measuring the experimental data only provides approximate information about the system due to observational errors, round-off errors, etc.

The process of identifying modelling errors is called validation, whose goal is to demonstrate that the mathematical model is a reliable representation of the real physical system. This step is performed after verification, the process of quantifying numerical errors (discretization, convergence, integration and coding errors) to check if the numerical solution is a good approximation of the analytical exact solution. The final step of verification often leads to accuracy assessment in order to reduce the numerical errors [12]. This thesis focuses on numerical errors, in particular, the estimation of the discretization error of the plasma-edge variables.

3.2 Discretization error

The discretization error $\epsilon_h$ is defined as the difference between the exact solution of the mathematical model $u$ and the exact solution of the algebraic system of equations obtained in the discretization, as the following expression shows:

$$\epsilon_h = u_h - u.$$  \hspace{1cm} (3.1)

A mesh with representative cell length $h$ is used for the solution of the discretized system $u_h$. The discretization error mainly depends on the discretization scheme used, mesh quality, and the behavior of the solution and its derivatives. Among the types of numerical errors, the discretization error is the most difficult to estimate as well as the most computationally expensive to obtain, since it normally requires solutions on different grid levels to be reliable [29]. Moreover, it is usually the largest source of numerical errors. A good rule of thumb is that the iteration error should be at least one order of magnitude smaller than the discretization error. The discretization error can be divided in two main components:

1. **Locally-generated**: the truncation error $TE_h$, which is defined as the difference between the discretized operator applied to the exact solution and the exact operator applied to the exact solution of the mathematical model. In other words, it is the error produced by the substitution of the mathematical operators of the differential equations with finite-scheme approximations. By using Taylor
3.3. Discretization error estimation methods

expansions, one can know how $TE_h$ scales with the reference mesh size $h$. The expression of the truncation error is:

$$TE_h = L_h(u) - L(u). \quad (3.2)$$

2. Transported from elsewhere in the domain, in a similar manner to the solution (e.g. for a convection-diffusion equation, the error will be convected and diffused from the regions where it is generated). [11].

This particular behavior is derived from the study of the error transport equations [29], that are obtained for linear operators when combining equations (3.1) and (3.2):

$$L_h(\varepsilon_h) = -TE_h, \quad (3.3)$$

where $L$ is a symbolic differential operator representing the PDE $(L(u) = 0)$, $L_h$ is a symbolic discrete operator representing the algebraic equation $L_h(u_h) = 0$ on a grid $\Omega_h$, and $u_h$ is the exact solution of the algebraic system on the grid $\Omega_h$ (continuum solutions must be restricted point-wise after discretization). As it can be observed in the discrete error transport equations (DETE), the $TE_h$ is the local error source for the $\varepsilon_h$ that is transported through the mathematical operator. In the case studied in this thesis, the operator corresponds to the plasma-edge differential equations that govern particle transport towards the divertor.

3.3 Discretization error estimation methods

Christopher Roy is considered one of the most authorized voices in the Computational Physics Community regarding numerical error verification and validation. In his work “Review of Discretization Error Estimators in Scientific Computing” [29], he gathers the most important methods developed by the scientific computing community in the topic of discretization error estimation, as well as how to verify the reliability in every case.

This section collects the most significant aspects of his work to have a general insight of error estimation for Finite Volumes (FV) and serves as a point of reference when discussing the most suitable estimation technique for the plasma-edge code in later sections.

There exist two types of approaches for estimating discretization errors:

1. **A priori estimating methods** are used for bounding the discretization error before the numerical solution. The main difficulty is bounding solution derivatives $C(u)$, which becomes in many cases the main cause for the method to fail.

$$\varepsilon_h \leq C(u) \cdot h^p. \quad (3.4)$$

2. **A posteriori estimating methods** are employed after the numerical solution is obtained. They are divided in two main groups:

   a) Higher-Order estimates methods.

   b) Residual-based methods.
3.3.1 Higher-Order methods

They compare the discrete solution to a higher-order estimate of the exact solution to the mathematical model. Besides, they only use information from the discrete solution (it is often required more than one solution in refined/coarsed meshes or different formal orders of accuracy).

1. Mesh refinement: Richardson Extrapolation

It employs three grids with a refinement factor between them to obtain an extrapolated solution of \( p + 1 \) order of accuracy. It is used for providing a discretization error estimate. In addition, if the estimate is very reliable, it can be used for correcting the fine mesh solution. The estimator of \( p + 1 \) order of accuracy of the exact solution to the mathematical model is:

\[
\bar{u} = u_h + \frac{u_h - u_{rh}}{r^p - 1},
\]

(3.5)

with \( p \) the order of accuracy of the discretization scheme and \( r = \frac{h_{\text{coarse}}}{h_{\text{fine}}} \). Only the solutions for two grids appear in Eq. (3.5), but the third grid is needed to estimate the order of accuracy \( p \) (see section 3.4.1).

Since the extrapolation is based on the order of accuracy of the underlying scheme, there are 5 related requirements to provide reliable estimates:

a) Asymptotic range for both discrete solutions.

b) Cartesian uniform meshes (In case of non-Cartesian meshes, it is required to perform transformations).

c) Coarse and fine meshes related through systematic refinement.

d) Smooth solutions.

e) Other sources of numerical error are small.

From the extrapolated solution \( \bar{u} \), the discretization error estimate is obtained:

\[
\varepsilon_h = u_h - \bar{u} = -\frac{u_h - u_{rh}}{r^p - 1}.
\]

(3.6)

This technique is suitable for any discretization method (finite differences (FD), finite volumes (FV), finite elements (FE),...) and it can be used for calculating any quantity of interest. However, reliability depends on several factors as well as the need of having multiple solutions in the asymptotic range. Therefore, it has a high computing cost.

2. Order refinement methods

These methods employ two or more discretizations on the same mesh but with different formal order of accuracy. Then, they combine these solutions to estimate the discretization error. One example of this technique is the Kutta-Feuhberg method [10]. The main drawback is that it is only easy to implement in FE.
3.3. Discretization error estimation methods

3.3.2 Residual-based methods

These methods use the discrete solution and additional information (mathematical model, discrete equations, sources of discretization error...). The calculation of the estimator is based on the truncation error (“residual”). There are three main types:

1. Discretization Error Transport Equations

   The discretization error is transported through the domain similar to the solution. There are two main approaches:

   - Continuous DETE (after linearization):
     \[ L(\varepsilon_h) = -TE_h(u_h), \]  
     with \( TE_h(u_h) = L(u) - L(u_h) \). It can be solved if \( TE_h \) is known or estimated.
   - Discrete DETE:
     \[ L_h(\varepsilon_h) = -TE_h(u), \]  
     it can be solved if \( TE_h \) is known or estimated.

   To approximate the \( TE_h \), one can follow two alternatives which correspond to the continuous or discrete approach:

   a) \( TE_h(u) = L_h(u) \) approximating the exact solution \( u \) with Richardson Extrapolation: \( u \approx u_{RE} \).
   b) \( TE_h(u_h) = -L(u_h) \). This alternative requires an intermediate step involving a continuum-to-discrete operator to evaluate the discrete solution \( u_h \).

2. Adjoint methods for system response quantities

   Adjoint methods are initially used for design optimization problems. Now, they are also used for estimating discretization errors of a system response quantity. The approximation of the discretization error in \( f(u) \) is:

   \[ \varepsilon_h = f_h(u_h) - f_h(u). \]  

   Then, employing Taylor expansions of \( f_h(u) \) and \( L_h(u) \) one obtains the following equation (discrete adjoint method):

   \[ f_h(u) = f_h(u_h) + \frac{\partial f_h}{\partial u} \big|_{u_h} \cdot \left( \frac{\partial L_h}{\partial u} \big|_{u_h} \right)^{-1} \cdot L_h(u). \]

   with the row vector of adjoint solutions \( \psi^T = \frac{\partial f_h}{\partial u} \big|_{u_h} \cdot \left( \frac{\partial L_h}{\partial u} \big|_{u_h} \right)^{-1} \). The adjoint variables are also called adjoint sensitivities (sensitivities of solution \( f_h \) to perturbations in \( L_h \)). In the second equation above, they also provide the sensitivity of error in \( f \) to the local sources of discretization error (i.e. the truncation error).

   The continuous adjoint method follows a similar analysis using expressions of \( f \) and \( L \).
3. Discretization error estimation

3.4 Reliability of discretization error estimation methods

Proving the reliability of an error estimator is indispensable to be able to complete numerical verification. Otherwise, all calculations cannot provide good confidence and are merely unproven predictions, and as a consequence, useless. Again, Roy discusses the requirements for reliability assessment in [29][22]. A summary of his work is presented below, which will be necessary to comprehend the results on plasma-edge error estimation of next chapter.

This section provides the steps that one must follow after the application of any of the estimation methods above. As it will be shown later, this phase adds a significant computational cost to the method applied since it always requires to demonstrate that the asymptotic range has been reached by calculating the observed order of accuracy. This process involves the use of several solutions on different refined meshes or with different orders of discretization schemes.

The most important requirement for reliability estimators is that the solutions must be in the asymptotic range. The concept of asymptotic range depends on the type of refinement used.

For discretization methods involving h-refinement, i.e. changing mesh resolution with different levels of cell size, the asymptotic range is defined as “the sequence of systematically-refined meshes over which the discretization error reduces at the formal order of accuracy of the discretization scheme” [29]. The Taylor expansion of the discretization error follows the expression:

\[ \varepsilon_h = c_p \cdot h^p + c_{p+1} \cdot h^{p+1} + c_{p+2} \cdot h^{p+2} + ... \]  (3.11)

The asymptotic range is reached when h is sufficiently small so that all higher-order terms combined in the Taylor expansion are negligible in comparison with the leading term. Outside this region, the behavior of the solution, and thus, the discretization error is unpredictable due to differences in the signs between higher-order terms (some terms may cancel each other, whereas other terms may add). One can confirm that the asymptotic range has been achieved when the observed order of accuracy matches the formal order of the discretization scheme. Therefore, the calculation of \( p \) is mandatory.

When p-refinement is employed, the asymptotic range is determined by examining the behavior of the numerical solutions with successively increasing the order of the discretization scheme, all on the same domain mesh. The formal order of accuracy is the theoretical rate of convergence of a numerical approximation of a differential equation to the exact solution, i.e. the theoretical rate at which the error is reduced as the mesh is refined.

On the other hand, the observed order of accuracy is the actual rate of error reduction with refinement, and thus, it provides the real behavior of the solution when the mesh is systematically refined, so it serves as a measure for testing reliability. Thereby, one can only trust the error estimate when the observed order of accuracy matches the formal order.
There are 5 basic requirements for the observed order to match the formal order and prove reliability of error estimates. These requirements coincide with those of Richardson extrapolation reliability, as the observed order of accuracy is directly employed in this estimation technique:

1. **All discrete solutions must be in the asymptotic range.** As stated before, this is an obvious requirement since it comes from the basic condition to confirm reliability. It should be highlighted that both fine and coarse meshes must be in the asymptotic range, i.e. if one of the meshes employed for calculating the observed order of accuracy is not in the asymptotic range, $p$ will not match the formal $p$.

2. **Uniform mesh spacing:** the discretization error expansion shows the dependency on a single mesh spacing parameter $h$. Since most of applications require non-isotropic meshes (i.e. non-cartesian), this condition would prevent this type of meshes. However, with the proper transformations that have at least the same order of the underlying discretization scheme, anisotropic meshes are allowed. Changes in mesh quality can severely deteriorate the order of accuracy, thus, these transformation should maintain sufficient grid regularity (stretching, aspect ratio, skewness, etc.)

3. **Systematic mesh refinement:** [22] requires that the mesh refinement be both uniform and consistent. Uniform refinement [28] requires that the mesh must be refined by the same factor over the entire domain. Consistent refinement [22] requires that the mesh quality must either remain constant or improve with mesh refinement.

4. **Smooth solutions:** discontinuities and singularities on the solution field reduces the order of accuracy in the region near-by, regardless of the method applied.

5. **Other numerical error sources must be small:** the presence of round-off errors, iterative errors, etc. will be amplified when calculating the order of accuracy, yielding unreliable values of it. It is usually a good rule of thumb, to have errors with two orders of magnitude smaller than the discretization error in the fine grid [28].

### 3.4.1 Observed order of accuracy?

There are two possibilities for calculating the observed order of accuracy depending on the grid refinement factor: (i) Constant grid refinement factor and (ii) Non-constant grid refinement factor. The grid refinement factor is defined as the ratio of reference spacing between two systematically refined meshes. In this thesis, only the case of constant refinement is considered for simplicity of implementation, since the non-constant case requires of a extra iterative procedure to obtain the order of accuracy.
3. Discretization error estimation

Therefore, the constant grid refinement factor reads as the following expression:

\[ r = \frac{h_2}{h_1} = \frac{h_3}{h_2}. \] (3.12)

Where \( h_1, h_2 \) and \( h_3 \) represent the reference cell size for the numerical solutions on a fine grid (\( \Omega_1 \)), medium grid (\( \Omega_2 \)) and coarse grid (\( \Omega_3 \)) respectively, and all of them with the same discretization scheme of \( p^{th} \) order of accuracy.

Assuming that the asymptotic range is achieved for all discrete solutions \( u_1, u_2 \) and \( u_3 \), the higher order terms in the Taylor expansions are neglected and only the leading term of order \( p \) remains yielding the observed order of accuracy:

\[ \hat{p} = \frac{\ln(u_3 - u_2)}{\ln(r)}. \] (3.13)

3.4.2 Additional remarks on reliability:

The five assumptions necessary for obtaining reliable estimates (i.e. for the observed order of accuracy match the formal order) are in some cases not enough to guarantee reliability: when applied to local quantities, that is when \( p \) is calculated point-wise in the domain, problems may appear under certain circumstances.

The first simple case occurs when part of the domain approaches the exact solution from above, whereas other part of the domain does it from below. At this crossover point (Figure 3.1), the observed order of accuracy will be undefined even for the hypothetical case of no discretization error at all.

Another case when local evaluation of \( p \) causes problems is provided by [27]. In this work, Roy tests an inviscid supersonic flow, formally a second order scheme
reduced to first order by flux limiters. However, he found oscillations in the observed order of accuracy and some other undefined values in the hyperbolic region. Therefore, local characteristics of the problem can also provide unreliable values for the observed order of accuracy.

### 3.4.3 Uncertainty estimators

In many applications, the problem of having results where the observed order of accuracy does not match the formal order, and thus, provides unreliable estimates, is very common in practical applications. Whether it caused by the failure of any of the reliability assumptions, in most cases it is due to the inability of obtaining solutions at the asymptotic range, as it may occur in many different situations (e.g. impossibility of sufficient refinement in certain regions, local characteristics that produce undefined order values, etc.).

However, this problem is fixable by converting the discretization error estimator into an uncertainty estimator. This epistemic uncertainties differ from aleatory uncertainties in that they are because of a lack of knowledge. Thus, they can be reduced by providing more information [22].

Techniques such as Grid Convergence Index proposed by Roache [26], and some extensions by other authors, provide a tool to solve the problem of unreliable estimates. This topic will be addressed with further detail in next chapter, when implementing the plasma-edge problem.

### 3.5 Applicability of methods to plasma-edge code: comparison and selection.

At this point, the tools for estimating discretization errors have been analyzed as well as the methodology that follows estimation, the reliability assessment. Now, the most suitable error estimation method for the plasma-edge case studied can be discussed.

The objective of this chapter is finding a suitable discretization error estimator for the plasma-edge code with a good compromise of the following 3 requisites:

1. **Accuracy**.

2. **Computational Cost**. Because of the complexity of plasma-edge problem, an extremely high computational cost is required for a single simulation. As a consequence, there exists an important restriction to the total number of cells since any estimating method involving refinement implies an increase of the number of cells affecting significantly the time employed for a simulation.

3. **Implementation cost**. Due to the complexity of the plasma code solver, any code-intrusive method will add a significant effort as well as it will be more prone to commit errors that affect the results.
3. Discretization error estimation

3.5.1 Discretization Error Transport Equations

This method provides in general lower accuracy than higher order methods and adjoint methodology. In addition, the accuracy of DETE depends mainly on the errors committed when estimating the source term, i.e. the truncation error. Nevertheless, it can be considered as a sufficiently accurate method when properly employed. It has to be remarked that it does not allow to calculate errors for response quantities (e.g. total heat flux at targets).

Regarding the computational cost, this technique implies solving the Discrete Error Transport Equations which have a similar cost as a forward simulation of the plasma code as they resemble very much (except source terms) and are solved with the same procedure. Theoretically, this technique is the cheapest computationally as it only requires one simulation. However, the exact solution to the mathematical model is not available and the derivation from the plasma equations is very complex, thus the truncation errors that acts as the source term in the DETE has to be approximated through other methods, adding significant cost to the original error estimation. One of the possibilities is estimate the exact solution by a finer mesh solution or by Richardson extrapolation and then insert it into the discrete operator. This requires at least an additional and more expensive forward simulation. Other options require a continuous projection of the numerical solution that requires the selection of piece-wise shape functions.

The implementation cost is the main drawback of this technique as it requires the derivation of the DETE in which the original plasma equations have to be adapted to include the different source terms and boundary conditions. Given the complexity of the original solver, this technique becomes one of the most expensive in terms of implementation cost.

3.5.2 Adjoint methodology

It is a very accurate method for estimating discretization errors. While most other methods are only capable of estimating the discretization error of the state variables, the adjoint method allows objective-oriented error calculation. One of the best advantages is that it provides the error sensitivities which can be used for adaptation.

Computationally-wise, it requires the solution of the adjoint problem on the same mesh which is of the same order of magnitude of a forward simulation of the plasma equations. Additionally, it can be observed in the expression 3.10 that it requires the approximation of the TE as happened for the DETE methodology. Therefore, at least three simulations are required: one forward with original mesh, one adjoint with original mesh and one forward with a finer mesh.

The derivation of the discrete adjoint equations is often quite complex in many engineering problems due to the difficulty of calculating the Jacobians. In this particular case, the complexity inherent to the plasma equations makes the task even harder such that in the original B2-Eirene code (Monte Carlo coupled to the FV solver) the feasibility would have to be proven.
3.5.3 Order refinement

Any comparison with a higher-order estimate of the exact solution always provides very high accuracy. P-refinement requires less computational effort than h-refinement as the number of cells is not increased with each refined mesh (the mesh size remains intact). Thus, two simulations of the same magnitude are necessary to obtain an estimate of the exact solution.

However, the implementation of this technique is code-intrusive as it consists of changing the discretization schemes of the solver, which have been carefully chosen for each convection, diffusion and source term of every plasma equation. The selection and implementation of suitable higher-order discretization schemes for all of these terms makes the implementation costly.

3.5.4 Mesh refinement: Richardson extrapolation

As a higher-order method, the accuracy of h-refinement is very high. It is suitable for finite volumes and it estimates the total error such that it can be used for quantities of interest. It employs three systematically refined meshes to obtain the extrapolated solution of higher order of accuracy, thus increasing significantly the computational cost of each simulation. Nevertheless, this method can employ coarser meshes for the extrapolation which have lower computational cost, whereas other methods require a finer mesh than the original one.

The low implementation cost is the greatest advantage of this technique as the original solver is not changed, and given the inherent complexity of the plasma equations this makes Richardson extrapolation one of the best candidates for estimating the discretization errors. The most difficult task is to perform adequately the reconstruction of refined solutions to the coarse grid points in order to calculate the extrapolation at the same points in the domain.

3.6 Summary of analysis and conclusions

The summary of the analysis it is provided in Table 3.1, from which the following conclusions can be extracted:

1. In principle, higher-order methods obtain a more accurate estimate of the discretization error whereas residual based methods achieve also high accuracy depending on the quality of the estimation of the truncation error. It is important to confirm that all steps that introduce errors to the final estimation are sufficiently small. For instance, the errors of the interpolation procedure to restrict solutions from a fine to a coarse mesh must be sufficiently small compared to the discretization error.

2. DETE methodology has the lowest computational cost in theory, but if high accuracy in the estimation of the truncation is desired, additional finer simulations are required such that the computational effort approximately matches adjoint and higher-order methods, which are of the same cost.
3. Discretization error estimation

The implementation cost therefore determines the choice of a particular method. In this regard it is clear that Richardson extrapolation is the easiest to implement in comparison to the other code-intrusive (DETE and p-refinement) methods or methods that require calculation of complex Jacobians (Adjoint methods).

<table>
<thead>
<tr>
<th>Methodology</th>
<th>Accuracy</th>
<th>Computational cost</th>
<th>Implementation cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>DETE</td>
<td>High</td>
<td>Lowest (if TE is available), but in this practical case:</td>
<td>Very high (code intrusive)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>High =</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>1 simulation (solve DETE) + 1 or 2 finer simulations to estimate TE</td>
<td></td>
</tr>
<tr>
<td>Adjoint Methodology</td>
<td>High</td>
<td>Very high =</td>
<td>Very high (Jacobians of system)</td>
</tr>
<tr>
<td>Order refinement</td>
<td></td>
<td>1 forward sim. + 1 reverse sim. + 1 or 2 finer sim. to estimate TE</td>
<td></td>
</tr>
<tr>
<td>Richardson extrapolation</td>
<td>Very high</td>
<td>Very high (3 simulations, but possibility to use coarser meshes)</td>
<td>Affordable</td>
</tr>
</tbody>
</table>

Table 3.1: Summary of applicability of discretization error estimation methodologies for the plasma-edge problem.

In each of the methods explained before, an estimation based on finer solutions is required either through the estimation of the truncation error (i.e. residual-based methods) or by the methodology itself (higher-order methods). Therefore, a reliability assessment based on the behavior of solution with refinement through the calculation of the order of accuracy is mandatory to check the confidence on the errors. This step is the differential reason to choose Richardson extrapolation over the other methods: for the reliability test it is essential to calculate the observed order of accuracy and check for which regions it does not match the formal order. Hence, three systematically refined meshes are required for this process, which is an intrinsic step in the Richardson extrapolation technique as the observed order of accuracy is calculated before extrapolation of solutions.

In addition, the feasibility of implementing RE to plasma problems has been already tested by [25] in which they successfully perform this technique on an equidistant uniform mesh with the goal of code validation, supporting the decision on h-refinement as the best option. This thesis aims the estimation of discretization error distribution over the domain on non-uniform meshes, which are more adequate to practical applications but require a deeper study on the reliability of estimates.

In conclusion, Richardson extrapolation is the most suitable discretization error estimation technique for the plasma-edge problem studied in this thesis.
In this chapter, complete Richardson extrapolation is applied to the plasma-edge model presented in Chapter 2, in order to accurately estimate the discretization error of different plasma variables. First, the algorithm to perform the extrapolation is discussed. Later in the chapter, the distribution of the error in the domain is analyzed for each case and the confidence of the calculated estimates is verified. Finally, a method for correcting non-reliable estimates associated with non-asymptotic behavior of solutions is provided.

4.1 Characteristics of the problem

The plasma variables selected for the error estimation are the ion density ($n_{\text{ion}}$) and ion temperature ($T_{\text{ion}}$), but this study could be extended to other plasma-edge variables. The physical domain corresponds to the slab test case (Chapter 2).

Figure 4.1 indicates the dimensions of the plasma-edge. The poloidal length $x$ of the domain is 10 m, while the radial coordinate $y$ extends from 2.5 to 2.6 m. To distinguish the different regions, the cuts and separatrix are shown in red. The cuts are located at 0.5 m from the targets and the separatrix is positioned at $y = 2.54$ m.

The discretization of the domain is achieved by generating a mesh with symmetric exponential refinement from the center towards the targets in the poloidal direction, called biased refinement. ($h_{i+1} = b \cdot h_i$, where $b$ is the “bias factor”).

This refinement is needed to capture accurately the steep gradients near the targets of several plasma state variables. To have a better perspective of the extreme nature of the plasma-edge state and to be able to discuss the results later in the chapter, plots of the ion temperature and ion density steady-state solutions are provided for a 70x20-grid with $b = 0.89$.

As it can be easily observed in Figure 4.2, the ion density presents a very flat profile in the center region (including core and scrape-off layer). On the other hand,
4. **Implementation of Richardson extrapolation in the plasma edge model**

**Figure 4.1:** Representation of the slab 2D domain with a biased refinement mesh toward the targets.

**Figure 4.2:** Solution of the ion density.

The combination of ions accelerating toward the targets and the ionization peak due to the interactions with the neutrals, lead to steep gradients in the vicinity of the target plates.

On the other hand, the ion temperature (Figure 4.3) has the greatest values in the core region (notice that only the outer layers of the complete core region are included in the plasma-edge model) which decrease significantly while approaching the SOL, yielding a strong gradient in the radial direction.
4.2. Implementation of the Richardson extrapolation algorithm

For the implementation of Richardson extrapolation in the Matlab Plasma Code to estimate the discretization errors of the ion temperature and ion density point-wise in the domain, it is required to have three converged solutions at three systematically refined meshes with a refinement factor between grids of 2. As presented before, the system of reference x-y corresponds to the poloidal-radial coordinates.

The following three meshes are employed to obtain the plasma state solutions: a coarse mesh with 70x20 cells, a medium 140x40 grid and a fine 280x80 grid. The discretization error of the finest grid will be calculated. It is important to highlight again the low number of cells for plasma-edge simulations in comparison to other numerical simulation applications. Figure 4.4 represents schematically the working of the algorithm.

4.2.1 Interpolation of the solutions to the coarse grid points

Since the solutions for the ion density and temperature are stored in the center of the cell volumes and these points do not coincide for the different refined grids, a method to rebuild solutions at the coarse grid centers is necessary. Two interpolation techniques are proposed:

1. **Interpolation method.** It interpolates the solutions from the medium and fine grids to the coarse grid points. Linear interpolation is used, which is a 2nd order accurate scheme and the order of the discretization scheme for the plasma edge model is expected to be smaller than 2. Any other higher-order interpolation scheme is allowed for this step, such as spline interpolation, which was also used in this step to verify the results.
4. Implementation of Richardson extrapolation in the plasma edge model

![Flow diagram of the Richardson extrapolation algorithm.](image)

**Figure 4.4:** Flow diagram of the Richardson extrapolation algorithm.

2. **Integration method.** It integrates the solution from the fine and medium cells to the coarse cell volume and then it averages the solution for this composite cell. (All guard cells have been neglected in the integration process). The integrals were approximated using the following integration rule, in which solutions are considered constant all over the cell domain:

\[
\bar{n}_{ion} = \frac{\int n_{ion} \cdot dV}{\int dV} = \frac{\sum n_j \cdot V_j}{\sum V_j}.
\] (4.1)

\[
\bar{T}_{ion} = \frac{\int T_{ion} \cdot dV}{\int dV} = \frac{\sum T_j \cdot V_j}{\sum V_j}.
\] (4.2)

Both methods are applied zone by zone, avoiding the interpolation or integration of values across the cuts.

A priori, the errors introduced in this step should be negligible compared to the discretization error if and only if the schemes used for integration or interpolation are at least the same order of accuracy or higher [12]. This is an important condition because in the later extrapolation of solutions, any noise measurement is amplified.

As mentioned in the last section, a combination of finite-difference schemes of 1\textsuperscript{st} and 2\textsuperscript{nd} order is employed. However, it is not possible to say that the order of a certain state variable is determined by the formal order of the single equation
which describes this state variable (continuity equation for the ion density, energy equation for the temperature...). As a system of coupled PDEs, the global order is determined by the overall system and should be around 1st order. Besides, in the region close to the targets the ions accelerate leading to a large convective part of the particle and energy flux, whereas the conductive heat flux becomes relatively small. Therefore, the dominance of the convective transport and upwind schemes is expected. Nevertheless, the exact order will be given by the calculation of the observed order of accuracy.

The interpolation and integration schemes used in this phase are higher than of the global order of accuracy of the system. As a consequence, these approximation errors are not expected to influence significantly the discretization errors.

4.2.2 Calculation of the observed order of accuracy

The general derivation for the observed order of accuracy \( \hat{p} \) is detailed in Chapter 3. For this particular case, it is obtained by the following expression at each coarse grid point:

\[
\hat{p} = \frac{\ln \left( \frac{u_{\text{coarse}} - u_{\text{medium}}}{u_{\text{medium}} - u_{\text{fine}}} \right)}{\ln(2)},
\]

(4.3)

where \( u \) corresponds to the state variable being extrapolated \( (n_{\text{ion}} \text{ or } T_{\text{ion}}) \). As commonly occurs in many applications, certain regions of the domain will have non-asymptotic behavior, yielding bizarre values for the observed order of accuracy such as complex, negative or even very high values compared to the formal order. To address this problem of unreliable estimates, upper and lower limits are set for the observed order calculations. If \( \hat{p} > p_{\text{formal}} \), then \( p \) is set to \( p = p_{\text{formal}} \). If \( p < 0.5 \) or undefined, then \( p \) is set to \( p = 0.5 \) [23]. A further detailed description of the non-asymptotic behavior problem along with techniques to provide reliable estimates is given later in the reliability study section (section 4.4).

4.2.3 Richardson formula

After the calculation of the observed order of accuracy, extrapolated solutions \( u_{RE} \) are determined from the Richardson expression:

\[
u_{RE} = u_{\text{fine}} + \frac{u_{\text{fine}} - u_{\text{medium}}}{2^{p} - 1}.
\]

(4.4)

Please note that this formula is evaluated at each of the coarse grid points in the domain, such that \( u_{\text{fine}} \) and \( u_{\text{medium}} \) come from the rebuilding phase.

4.2.4 Discretization error estimates

Finally, the last step in the algorithm corresponds to the actual aim of the whole process: to obtain the distribution of discretization error over the domain. Again,
the extrapolated results are employed point-by-point in the coarse grid to obtain the absolute and relative discretization errors:

\[ \varepsilon_h = u_{\text{fine}} - u_{\text{RE}}. \]  

(4.5)

\[ \varepsilon_h(\%) = \frac{u_{\text{fine}} - u_{\text{RE}}}{u_{\text{RE}}} \cdot 100\%, \]  

(4.6)

where \( u_{\text{fine}} \) is the fine solution restricted to the coarse grid points. It is also possible to get back to the fine grid with a simple interpolation to find the discretization errors at the original fine mesh.

4.3 Results

In this section, the results for the discretization error estimates obtained with the algorithm presented above are provided and analyzed. The integration methodology for restricting solutions to the coarse grid centers is employed.

Since a final and necessary step to convert the errors into uncertainty estimates will be performed later in the chapter, only a quick analysis of error distribution is aimed in this section, whereas the complete quantitative analysis will be done in a later section. It is important to remark, that the results were obtained point-by-point in the domain (corresponding to the location of the coarse grid centers), but the representation is given in a continuum interpolated colormap to better understand the distribution.

4.3.1 Discretization error estimates for ion density

In Figure 4.4, results for the relative discretization error (\%) of the ion density are represented in two different perspectives to be able to recognize the regions of highest errors. The upper figure provides a 3D surface of the error distribution in the domain, which facilitates to locate the region of highest error concentrated in a very narrow layer on the targets, difficult to perceive in the 2D colormap perspective (lower figure). On the other hand, the later perspective is more suited to detail the error distribution with precision in each region of the 2D domain. Because of the symmetry of the plasma solutions studied, the errors will follow a very symmetrical profile.

The highest discretization errors are concentrated at the targets of the scrape-off layer (red in colormap). They cover all the target region extending radially with some peaks in the middle part and then decreasing towards the separatrix. In the private flux region, they increase but with lower values than the SOL.

Moving apart from the targets, the errors drop significantly to very low values (blue in colormap). It can be noticed local maximums (green in colormap) situated in the SOL next to the X-point (intersections between cuts and separatrix).
4.3. Results

4.3.2 Discretization error estimates for ion temperature

The relative discretization errors (%) for the ion temperature are presented in the same manner as the ion density, with a 3D surface and 2D perspective to easily find error differences.

In this case (Figure 4.5), the global maximum relative errors are located in the private flux region very close to the X-point. The targets (in the SOL and private flux region) again show in general higher errors than the rest of the domain, particularly bigger in the middle part of the SOL targets (green in colormap), as well as the SOL points close to the X point that extend along the separatrix. The inner part of the SOL predicts low relative errors, while the core region has the lowest errors of the whole domain.

Figure 4.5: Relative discretization error (%) of the ion density in 3D and 2D perspectives.
4. Implementation of Richardson extrapolation in the plasma edge model

4.4 Reliability analysis

The discretization error estimates of previous section provide a first approximation to the real discretization errors. However, a correcting procedure was applied to the observed order of accuracy by setting upper and lower limits in order to avoid behavior far from the global order as well as to not underestimate errors. As a consequence, some regions may not be reliable and a reliability study of these points has to be done to make further adjustments to improve the confidence on the error estimates, such as converting the errors into uncertainty bands as a final step.

Therefore, the next step is the analysis of the calculated observed order of accuracy in every point of the domain, which gives information about how the solutions behave with refinement for this particular type of mesh.
4.4. Reliability analysis

4.4.1 Cases of non-asymptotic behavior

At points in which the observed order of accuracy is very distant to the formal order, the solution exhibits some type of non-asymptotic behavior: it may never converge with refinement (undefined and negative values), it will converge very slowly (near to 0 values) or the error will be underestimated ($\hat{p} \gg p_{formal}$). In Table 4.1, the behavior of the solution with refinement is detailed depending on the value of $\hat{p}$:

<table>
<thead>
<tr>
<th>Convergence</th>
<th>Order</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oscillatory</td>
<td>$\hat{p} = undefined$</td>
</tr>
<tr>
<td>Diverging (very slow)</td>
<td>$\hat{p} &lt; 0$</td>
</tr>
<tr>
<td>Converging</td>
<td>$0 &lt; \hat{p} &lt; p_{lower}$</td>
</tr>
<tr>
<td>(under-estimation of error)</td>
<td>$p_{formal} &lt; \hat{p}$</td>
</tr>
</tbody>
</table>

Table 4.1: Behavior of solutions depending on the observed order of accuracy [23]

Therefore, all these points will provide unreliable estimates. The problem of non-asymptotic behavior is very common in many engineering applications that address complex problems, especially in CFD, and has its origin in the type of discretization applied to the problem and the characteristics of the problem itself [29]. Since error estimates are still desired for this regions, the common first step is setting thresholds to the observed order of accuracy in order to force the extrapolated solution to follow a behavior closer to the formal order, as performed in the algorithm.

The limits selected for this particular problem are:

- the upper limit $p_{formal} = 1$, which corresponds to the expected formal global order (in some cases it could change over the domain depending on each variable, but a conservative approach sets the order to the minimum of possible orders to never underestimate the error).

- the lower limit is set to 0.5 as it is recommended in [23]. This latter value can be decreased down to 0.1.

The following figures illustrate the observed order of accuracy in the 2D Slab domain calculated for the ion density and ion temperature. The interpolated colormaps provide a continuum representation of the point-wise values. All values corresponding to non-asymptotic behavior (oscillating or diverging) are set to zero (dark blue in colormaps).

Regarding the observed order of accuracy of the ion density for the biased grid (Figure 4.6), multiple areas predict non-asymptotic behavior: (i) a big area in the central region covering both SOL and core; (ii) areas in the top part of divertor legs that extend along targets but improve when approaching the separatrix; (iii) next to the x-point in the SOL; (iv) in the plane parallel to $y = 2.5$ m.
4. Implementation of Richardson extrapolation in the plasma edge model

Additionally, certain points present peaks with very high values far from the global order (values up to 5 units approx.). These behavior happens usually next to non-asymptotic solutions under certain local characteristics of the problem. For instance, in the SOL zone next to the X-point, non-asymptotic values appear along with local peaks, yielding a non-reliable zones for estimates. The orders in rest of the domain (values close to 1 (light blue in colormap)) are expected to be reliable.

![Distribution over the 2D domain of the observed order of accuracy of the ion density for the biased grid.](image)

**Figure 4.7:** Distribution over the 2D domain of the observed order of accuracy of the ion density for the biased grid.

On the other hand, Figure 4.7 provides the results for $\hat{\rho}$ of the ion temperature. In comparison with the other variable, the observed order of accuracy is not deteriorated in most part of the domain and presents values very close to the formal order, yielding good estimates.

Non-asymptotic behavior accompanied by high peaks occurs only in the SOL targets in a region very close to the separatrix. Besides, a region with very slow convergence appears close to the X-point along the separatrix in the SOL.

4.4.2 Analyzing causes for non-asymptotic solutions

There are different possible causes for obtaining deteriorated values of the observed order of accuracy. First of all, it is necessary to check if there is a violation on any of the five basic requirements for the observed order to match the formal order and prove reliability of error estimates [29]. The study of each of the five assumptions for reliability is presented below starting from the clearest points to those ones that have to be further analyzed:

1. **Are other numerical sources of error small?**

   This point is clear since the solutions for the three refined meshes have residuals of order $10^{-8}$. Besides, errors introduced in the process of restricting solutions to the coarse grid points are minor. Therefore, the requirement is met.
2. Are the solutions smooth?

Even though the domain presents apparent discontinuities due to the cuts, in reality the cut configuration does not produce discontinuities in the state variables as it is only employed for simplifying the representation of solutions. In addition, there is no existence of shocks as the speed of sound is only reached at the target plate, which is imposed as a boundary condition. In the remainder of the domain the flow is always subsonic. There are not any singularities present in the plasma field.

3. Is the refinement between the 3 meshes systematic?

For obtaining finer meshes, the procedure employed was splitting each cell in both directions, doubling the number of poloidal and radial cells fulfilling uniform refinement condition. On the other hand, the mesh quality between grids is maintained as the aspect ratios, stretching factors and other grid parameters remain intact. Therefore, systematic refinement is achieved.

4. Are cells fine enough to reach the asymptotic range?

This is probably the key requirement to reach the asymptotic range and it is also one of the most difficult to achieve at certain conditions of many problems. It is required that the 3 meshes involved in the extrapolation are all in the asymptotic range. The exponential refinement was chosen in order to capture accurately the regions with highest gradients and thus, achieve enough refinement to guarantee the asymptotic range in terms of cell size.

However, certain characteristics of the problem itself can cause the failure of reaching the asymptotic range regardless of the degree of refinement as it is detailed later.
5. Is the mesh sufficiently uniform?

Non-uniformity is allowed if there is enough grid regularity to preserve mesh quality. The biased grid configuration is very precise but at the cost of having great differences in the aspect ratios (the aspect ratio is large in the core and smaller near the targets). In addition, there is a great change of the poloidal length of subsequent cells near the targets. Therefore, grid irregularity is likely one of the main reasons for deteriorating the order of accuracy.

Another important aspect is how the cell size varies along the poloidal direction: it is necessary to have a smooth size variation between consecutive cells to conserve the order of accuracy close to the formal value.

Therefore, the exponential refinement toward the targets may have problems in fulfilling the requirements of mesh regularity and quality, and as a consequence, causes the deterioration of the observed order of accuracy.

The ideal mesh should have a high degree of accuracy and mesh regularity, as a fine uniform grid, that achieves very small discretization errors and minimizes at the same time the regions where $p$ is deteriorated. The perfect candidate would be a very fine and uniform grid. However, such a fine uniform mesh gives rise to an enormous computational cost due to the high number of grid cells. This type of configuration might only be possible in very simplified versions of the plasma problem, such as 1D cases in only one zone.

Therefore, in practice one must pursue mesh configurations that favor one of the requirements in detriment of the other. In fact, the biased grid constitutes a perfect example of leaning towards high accuracy at a cost of low mesh quality. The opposite case of opting for good mesh quality would be a completely uniform but coarse grid, which captures badly the solution variations and could have regions outside of the asymptotic range. Between these two cases, there exist configurations that are a good compromise between refinement and regularity.

In order to test one of these possible configurations, it was selected a grid divided into two zones with different level of equidistant poloidal refinement (divertor legs and core region). Both regions were joined by a smooth transition defined by a bezier curve. To perform Richardson extrapolation, solutions for three systematically refined meshes of 180x10 cells, 360x20 cells and 720x40 cells were employed. The number of cells was selected aiming to have approximately uniform cells as well as having a similar number of cells as the biased grid case. To picture better the grid configuration, the coarse grid is presented in Figure 4.8. Note that the zone that is faded to black is an equidistant mesh that cannot be pictured properly in detail due to the high amount of small cells (also it is not in real scale).

The results for the observed order of accuracy for the new bezier grid configuration are summarized in Figure 4.9 and Figure 4.10.

For the ion density case, it can be noticed by simple inspection that the central region of non-asymptotic behavior has dissapeared with the new more uniformed cells. Instead, results suggest that schemes of 2nd order dominate in this zone, and downgrade while approaching the boundaries of the SOL. As explained before, it is
4.4. Reliability analysis

Figure 4.9: Representation of the slab 2D domain with two regions of different equidistant refinement and a bezier curve transition in between.

Possible that the global order for this variable is not 1st order all over the domain, as expected because of convective fluxes predominance. However, the conservative approach suggest to maintain 1st order as the global order ensures that the error will not be under-estimated in any case. In the outer regions of the SOL and core, the non-asymptotic behavior remains very similar as the biased grid case, except a remarkable improvement very close to the targets, yielding values that show good convergence.

Figure 4.10: Distribution over the 2D domain of the Observed order of accuracy of the ion density for the bezier grid.

For the ion temperature case, the non-asymptotic points have dissapeared and only remain points of slow convergence. However, the appearance of a peak alongside
4. Implementation of Richardson extrapolation in the plasma edge model

A low value could be considered as non-reliable. In general, the observed order is of 1st order as predicted.

![Observed Order of Accuracy of Ti (bezier grid)](image)

**Figure 4.11:** Distribution over the 2D domain of the Observed order of accuracy of the ion temperature for the bezier grid.

As it can be seen, the regions of non-asymptotic behavior have disappeared for the ion temperature and have been drastically reduced for the ion density in comparison to the biased grid, as well as the accuracy is closer to the formal order in most part of the domain. In conclusion, the observed order of accuracy has been improved for both state variables as expected, confirming the hypothesis that the mesh quality plays a very important role in determining the order of accuracy. However, there are still regions that suggest non-asymptotic behavior or combination of high peaks and low values next to each other (also non-reliable behavior). These particular cases might be caused by insufficient refinement or even by local characteristics of the problem.

The influence on the discretization error by the improved order of accuracy of the bezier grid will be discussed in next section when calculating the uncertainty final estimates, which will provide the conclusions of which grid is more suitable for the plasma-edge model.

### 4.4.3 Local characteristics of the problem

However, even if the requirements of mesh quality and enough refinement are successfully satisfied, non-asymptotic behavior can still occur depending on the characteristics of the problem itself. As explained in Chapter 3, at points where the 3 refined solutions cross each other, the behavior of the solution is undefined. Additionally, local characteristics can cause high oscillations in the order of accuracy from one cell to its neighbor affecting all the region nearby, thus providing unreliable estimates.
A particular important case is oscillatory convergence. In [6], it is demonstrated that this type of non-asymptotic behavior may occur when mixed order discretization schemes are employed and when certain coefficients of the discretized equations present highly oscillatory behavior as well. “A usual source for these variations is the oscillatory velocity that appears at recirculation regions near separation and reattachment points”.

Additionally, the paper shows that there exist a great amount of discretization schemes that exhibit oscillatory convergence, even in the asymptotic range. It is commonly argued that in the asymptotic range, the leading term of the Taylor series expansion of the solution always dominates over the higher order terms. However, this argument is wrong because it assumes that higher-order derivatives become small as \( h \) approaches 0, which does not occur in many cases depending on the discretization scheme. In fact, for upwind methods and mixed-order methods these derivatives are discontinuous. This is particularly proved in the paper for the case of a convection-diffusion equation that uses mixed-order methods as upwind scheme along with central differences.

The scrape-off layer plasma problem of this thesis gathers exactly the conditions exposed above:

1. The discretization schemes are a combination of upwind, central and hybrid schemes, i.e. mixed-order schemes.

2. The PDE system is based on convection-diffusion type equations with recirculation regions.

Therefore, it can be assumed that oscillatory convergence may appear at different locations of the domain. It is straightforward to prove oscillatory behavior by representing the profile of the three refined solutions at the suspected regions (i.e. with observed order of accuracy undefined or complex). In the case of monotonic convergence, the solution of the medium grid should always be in between the fine and coarse grid solutions. Otherwise, the solution is oscillating. With the goal to assess the convergence behavior of the state variables on these problematic regions, different solution profiles for the 3 meshes were plotted together. In these plots, the medium solution profile did not appear in between, proving the non-asymptotic convergence predicted in the observed order of accuracy calculations.

### 4.5 Uncertainty GCI method to solve non-asymptotic behavior

It is very difficult to select a grid that fulfills all requirements without the detriment of the others or may even not be possible for the problem itself. Therefore, non-
4. Implementation of Richardson extrapolation in the plasma edge model

Figure 4.12: Plot of the three refined solutions for ion temperature in the poloidal plane \( y = 2.543 \) m to prove oscillatory behavior.

Asymptotic behavior may occur in most of the grid configurations for the plasma-edge model. However, reliable discretization error estimates are still desired for the regions where the observed order of accuracy does not match the formal order. One method to achieve reliable estimates was introduced in section 3.4.3, which consists in converting the error into an uncertainty estimator.

The Grid Convergence Index method was initially proposed by Roache [26] and has been further developed by other authors, such as the GCI with recommendations of Oberkampf and Roy. The application of this method constitutes the final step to obtain reliable discretization error estimators for the ion density and ion temperature in the plasma-edge model. It will be tested for the biased grid and bezier grid configurations, to be able to compare the resolution of both meshes and the influence of the observed order of accuracy.

4.5.1 GCI method with recommendations from Oberkampf and Roy

Oberkampf and Roy [22] provide an uncertainty estimator (labeled \( \varepsilon_{\text{GCI-OR}} \)) in which the Factor of Safety is defined depending on the observed order of accuracy. The Factor of Safety, abbreviated as FS, allows to define the chance that the true error will be inside the estimated error band. According to Roy [29], “there is an equal chance that the true exact solution is above or below the estimated value. Thus a factor of safety of \( FS = 1 \) centered about the fine grid numerical solution \( u_{\text{fine}} \) will only provide 50% chance that the true error is within the error band. Increasing the factor of safety should increase the confidence that the true error is within the error band”. A \( FS = 3 \) will provide a 95% chance that the error will be in the error band.

The \( \varepsilon_{\text{GCI-OR}} \) is calculated as the absolute value of the discretization error estimate multiplied by FS, which takes a value of 1.25 for those \( \hat{p} \) that are very close to the formal order (within 10%) or a value of 3 for results with \( \hat{p} \) outside from the
10% of the formal order, which are less reliable and need to ensure that the error is not underestimated and it is inside the error band.

\[ \varepsilon_{GCI-OR} = FS \cdot | \frac{u_h - u_{rh}}{r_p - 1} |. \]  
(4.7)

For \( \hat{p} \) within 10% of \( p_{formal} \):

\[ FS = 1.25 \quad \hat{p} = p_{formal}. \]  
(4.8)

For \( \hat{p} \) outside 10% of \( p_{formal} \):

\[ FS = 3 \quad \hat{p} = \min(\max(p_{low}, \hat{p}), p_{formal}), \]  
(4.9)

where \( p_{low} \) is the lower limit, which it is recommended to be set to 0.5 [23].

4.5.2 Results: GCI discretization error estimates

After applying the GCI methodology, the discretization errors for the ion density and ion temperature calculated in last sections are converted into uncertainty errors, that will provide a good confidence that the true discretization error is within the error band.

**Bias grid case: Fine mesh 280x80 cells.**

The highest discretization errors are concentrated in the targets of the scrape-off layer (red in colormap). They cover all the target region extending radially with some peaks in the middle part and then decreasing towards the separatrix. In the private flux region, they increase but with lower values than the SOL.

Regarding the GCI discretization errors of the ion density (Figure 4.12), the highest errors are still concentrated at the divertor targets on the scrape-off layer (red in colormap). Moving down the targets region from the most external radius \( y = 2.6 \) m, relative errors are found around 5% with a global peak near the middle part of the targets of value 5.25%. Then, the error decreases while approaching the separatrix to increase again in the private flux region up to values between 3% and 4%. Moving appart from the targets towards the central regions of the domain, rapidly the errors drop to very low values (blue in colormap). In this transition, the divertor legs still show errors between 2% and 3%. In addition, local maxima of 2.75% (green in colormap) appear in the SOL next to the X-point (intersections between cuts and separatrix). A slight increase in the central region of the SOL has values of 0.5%. Finally, the core region presents very low errors close to 0.01%.

The main reason why the biggest discretization errors are found at the divertor targets is a combination of different factors:

- The most influencing factor is that even the extreme refinement achieved at this region by the biased configuration, the ion density gradients are so big that they make it very difficult to capture the details of the plasma profile

- The non-asymptotic behavior or very slow convergence of these regions makes the error to not be reduced rapidly with refinement.
4. Implementation of Richardson extrapolation in the plasma edge model

- The less reliability forces to employ factors of safety to improve the confidence, a process that increases significantly the total error.

![Figure 4.13: GCI-OR Relative discretization error (%) of the ion density with biased grid configuration in 3D and 2D perspectives.](image)

Regarding the GCI discretization errors of the ion temperature (Figure 4.13), a slightly different distribution of error appears in comparison with the regular case without GCI conversion (Figure 4.5), but still concentrating highest errors around the X-point. A new global maximum with steeper profiles is located in the private flux region near the X-point with a value of 10.4%. The next biggest error is located in the core region right in the X-point, showing a relative uncertainty error equal to 8.7%. In the SOL, it can observed that errors of 6.5% extend from the X-point along the separatrix towards the center region. The rest of the divertor legs transitions from a peak in the targets of 7.8% to the center with errors rounding 4% (light blue in the colormap). The inner part of the SOL predicts again low relative errors, while the core region has the lowest errors of the whole domain.
4.5. Uncertainty GCI method to solve non-asymptotic behavior

In this case, errors predicted are very reliable even before the application of FS, since the observed order of accuracy was very close to the formal order in mostly the whole domain, only showing non-asymptotic behavior in a narrow region in the SOL along the separatrix starting from the targets (recall Figure 4.7).

![Graph showing GCI-OR Relative discretization error (%) of the ion temperature with biased grid configuration in 3D and 2D perspectives.](image)

**Figure 4.14:** GCI-OR Relative discretization error (%) of the ion temperature with biased grid configuration in 3D and 2D perspectives.

**Bezier grid case: Fine mesh 720x40 cells.**

At this point, it is clear that the Bezier grid configuration was chosen to test the influence of mesh quality on the order of accuracy. In last section, it was concluded that the uniformity of this type of mesh led overall to an improvement in the order of accuracy compared to the biased mesh. However, the influence on the discretization error still has to be discussed.

As it can be seen in Figure 4.14 and Figure 4.15, which describe the GCI-OR relative discretization error for the ion density and ion temperature in the bezier grid, the distribution of error remains almost identical with the highest errors at the divertor targets and X-point respectively. However, these errors have become
4. Implementation of Richardson extrapolation in the plasma edge model

totally inadmissible reaching values of 40% for the ion density and 25% for the ion
temperature. On the other hand, the errors in the central region are also very low
as in the biased case. Therefore, the improvement in reliability by improving the
observed order of accuracy does not translate into reduction of the discretization
errors since the mesh resolution in these regions is completely insufficient.

Figure 4.15: GCI-OR Relative discretization error (%) of the ion density with
bezier grid configuration in 3D and 2D perspectives.

4.6 Conclusions

In this chapter, the Richardson Extrapolation methodology was succesfully applied
to the plasma-edge model in order to estimate the distribution of discretization
4.6. Conclusions

Figure 4.16: GCI-OR Relative discretization error (%) of the ion temperature with bezier grid configuration in 3D and 2D perspectives.

error of the ion density and ion temperature over the 2D Slab case domain. The domain was discretized with two types of meshes: (i) a “biased grid” with exponential refinement towards the divertor targets and (ii) a “bezier grid”, comprised of two zones with different levels of equidistant poloidal refinement (divertor legs and core region) smoothly joined by a bezier curve transition.

The method employed in the algorithm to rebuild solutions at the coarse grid points was an integration procedure, which fulfills the condition of employing schemes with higher order of accuracy than global order, to neglect the introduction of other errors (The global order is expected to be 1st order mainly because of the dominance of convective transport and upwind schemes).

The analysis of the observed order of accuracy for each variable in the biased grid case revealed that several regions in the domain presented slow convergence with refinement or even non-asymptotic behavior, providing low reliability of the error estimates in these zones. It was suspected that the low mesh quality of the biased grid
4. Implementation of Richardson extrapolation in the plasma edge model

(very high aspect ratios) was responsible of this behaviors. For this matter, the bezier grid configuration was tested resulting in a great overall improvement of the observed order. However, there were still some regions with slow convergence and asymptotic behavior, that may be explained with insufficient refinement or even caused by local characteristics of the problem itself, such as the oscillatory behavior that can occur when combining mixed-order schemes in a convection-diffusion equation.

In order to fix the reliability problem associated with slow convergence and non-asymptotic behavior, the discretization errors were converted into uncertainty errors by the GCI method with recommendations of Oberkampf and Roy. This technique allows to improve the confidence by calculating error estimates with 95% chance that the true error will be inside the uncertainty error band. After applying it to the biased grid and bezier grid cases, the distribution of GCI-OR discretization error was finally obtained for each plasma state variable at each case.

Regarding the ion density of the biased grid configuration, the highest relative errors were concentrated at the divertor targets in the scrape-off layer, yielding values around 5%. This is explained by the difficulty even for the extreme refinement of the biased grid to capture the enormous gradients at this region, in addition with the slow convergence or even non-asymptotic behavior. The private flux region presented errors between 3% and 4%. Moving apart from the targets towards the central regions of the domain, rapidly the errors dropped to very low values. Regarding the ion temperature, maximum relative errors (8.7% - 10.4%) were located near the X-point. In the SOL, it was observed that errors of 6.5% extend from the X-point along the separatrix towards the center region. The rest of the divertor legs transitioned from a peak in the targets of 7.8% to the center with errors rounding 4%. The inner part of the SOL predicted low relative errors, while the core region has the lowest errors of the whole domain. On the other hand, the bezier grid results showed a similar distribution of error but with inadmissible errors (up to 40% for the ion density and 25% for the ion temperature) confirming that the improvement in the order of accuracy does not justify the selection of this mesh because of its poor mesh resolution for the plasma-edge problem.

However, it is remarkable that since it predicts better the order of each variable, it can help to estimate with more precision the global order of each region and state variable. This means that new higher limits for the order of accuracy could be set that lead to error reduction at some regions (thanks to the order itself and by applying a lower Factor of Safety in the GCI-OR). Nevertheless, since it is difficult to prove the real global order, the most conservative approach suggests to set the order to the smallest of all possible orders of the discretization schemes used (in this case 1st order) such that the errors are never underestimated.

Finally, it can be concluded that the biased grid configuration is a good solution to capture the extreme nature of the plasma-edge and obtain admissible relative discretization errors in comparison to other more uniform meshes.
Chapter 5

Mesh adaptation for discretization error reduction

The second stage of the thesis, which aims finding a mesh adaptation method for reducing the discretization errors, begins in this chapter. First, the possible mesh adaptive techniques are introduced. Up to this point, a complete method for estimating the discretization error distribution based on Richardson extrapolation has been presented and applied to the plasma-edge problem studied in this thesis. However, mesh adaptation algorithms require to estimate the error distribution multiple times (i.e. every time the mesh configuration is changed) and thus, other important factors as the computational cost may have a bigger impact. In that sense, other error sensors with different properties to guide the adaptation process have to be analyzed in order to choose the most suitable. Therefore, a literature review about the so-called error indicators is performed in the chapter to obtain the best candidates.

5.1 Mesh adaptation techniques

In the CFD community and especially in aerospace and aeronautics engineering, several authors have developed methods for finite volume adaptation algorithms in order to improve the accuracy of flow calculations. A general classification of these Adaptive Mesh Refinement (AMR) techniques is the following [14]:

1. r-refinement. It consists of a redistribution of cells towards regions of higher errors without increasing the total number of cells. Design optimization problems can be considered in this category.

2. h-refinement. It consists of splitting cells to refine regions of large error or removing faces to coarse regions of low errors, in an effort to improve the accuracy only on areas where is actually necessary. Nevertheless, the total number of cells is usually increased and consequently the computational cost of the adaptive strategy.
3. **p-refinement**: This technique consists of increasing the order of accuracy of the discretization schemes. Therefore, higher-order discretization schemes along with bigger stencils are used for rebuilding the solver.

Combinations of the refinement strategies are always possible, such as hp-refinement or hr-refinement, but with a significant increase in implementation cost. For this thesis, just the first two methods will be taken into account since p-refinement requires the adaptation of the solver and data structure. It is important to remind that the plasma model implemented in the Matlab code has a structured grid approach. Therefore, any strategy must avoid the appearance of hanging nodes (typical in unstructured grids) that force to change the data structure and solver.

### 5.2 Error sensors to guide adaptation

The first step in any adaptation algorithm with error reduction purposes is to find a suitable error sensor, usually called error indicators. A literature review in this topic is provided by Fraysse [13][14], who compares the most important error indicators including the their application to CFD problems, which is reproduced here to serve as reference for the plasma-edge problem discussion. The original references and mathematical formulation will be kept also for convenience.

The error indicators can be classified in two big families: (i) feature-based error indicators and (ii) numerical-based error indicators.

#### 5.2.1 Feature-based error indicators

A classical approach for adaptation is using parameters based on physical features, i.e. which rely on the solution profile of each variable. There are several types of feature indicators that have been tested successfully. The most common are (i) gradient detectors, which are calculated at each cell by evaluating the gradient difference between its edges and (ii) difference detectors, which are derived from the differences in the solution profile among the different faces of each cell.

The derivation of a feature-based indicator is very simple and computationally cheap, since it only requires a single simulation on the current mesh. For instance, a difference detector is defined at all edges of each cell by the following expression:

\[
\Delta \phi_i = | \phi_i(x_{p1}) - \phi_i(x_{p2}) |,
\]

where \(i\) corresponds to the face adjacent to cells centered in \(x_{p1}\) and \(x_{p2}\). Then, the indicator is normalized with the maximum value of the domain. This strategy usually works well with h-refinement methods by setting thresholds that help the algorithm to decide whether to refine or not. If the indicator is above the threshold, the face is bisected. There are other cell difference detectors with similar approaches for decision-making such as setting upper and lower limits to decide to split a cell in two or remove a face to make it coarser [19].

These error sensors allow to locate flow phenomena, such as regions of large gradients, shocks, etc. which are often associated with the largest errors. The main
advantage of these error sensors is the low computational effort required in every step of an h-refinement adaptative algorithm. On the other hand, these parameters do not include the behavior of the solution with refinement and are not directly related to discretization errors, resulting in a low reliability of the error localization. “Their lack of mathematical foundation makes them difficult to apply (...) to problems far from established experience” [14]. Finally, increasing the resolution of regions based on feature detectors does not necessarily lead to an improvement in the accuracy of quantities of interest [1].

The application of difference detectors to a scrape-off layer plasma with unstructured grids and some initial regularity plasma has been performed by [19], yielding good results in improving the accuracy. However, it still has to be proved for structured grids with extreme refinement as the bias grid. Consequently, difference detectors are considered as one of the possible candidates for mesh adaptation, and will be tested later in this chapter.

5.2.2 Numerical-based error indicators

Unlike feature-based indicators, the family of numerical-based error indicators does not provide the unreliability associated to the lack of mathematical foundation, as they provide the estimate of the actual discretization error. The so-called residual-based adaptation indicators are divided in truncation error and discretization error estimators, that can be grouped in three methodologies: (i) Adjoint-based adaptation indicators, (ii) $\tau$-estimation and (iii) Richardson extrapolation indicators.

Adjoint-based error indicators

The adjoint methodology can be used for estimating discretization errors, but the real advantage is that it can be used to obtain an error sensor for improving the accuracy of quantities of interest (e.g. the heat flux in the divertor targets).

These global outputs are for instance obtained by an surface integral of a variable field. By discretizing the system of partial differential equations, the global output can be also expressed in discrete form as $J_h(U_h)$. Venditti and Damorfal [30] developed the complete derivation of adjoint-based error sensors including the mesh adaptive strategy. The resulting discretization error is expressed as:

$$J_{h_f}(U_{h_f}) - J_h(U_h) \approx (J_{h_f}(\hat{U}_{h_f}) - J_h(U_h)) - \Psi_{h_f}R_{h_f}(\hat{U}_{h_f}),$$ (5.2)

where $h_f$ is the fine grid, $R_{h_f}(\hat{U}_{h_f})$ refers to the discrete equations evaluated with an approximated solution $\hat{U}_{h_f}$ obtained by an interpolation procedure from the current mesh solution $U_h$. The adjoint solution vector is obtained from a discrete linear system:

$$[\Psi_{h_f}]^T = \frac{\partial J_{h_f}}{\partial U_{h_f}} \frac{\partial R_{h_f}}{\partial \hat{U}_{h_f}}^{-1}.$$ (5.3)
Following the derivation, Fraysse proposes an error indicator $I_i^{hf}$ for each cell of the fine mesh, which has to be interpolated back to the current mesh:

$$I_i^{hf} = |((\partial \Psi_{hf})_i^T \mathbf{R}_{hf}(\tilde{U}_{hf}))|,$$  \hspace{1cm} (5.4)

where $\partial \Psi_{hf} = \Psi_{hf} - \Psi_{hf}$ which is approximated again by an interpolation procedure, to avoid computing the expensive fine adjoint solution. This discretization error estimation allows either to use h-refinement strategy with thresholds or design optimization.

The aim of this thesis is reducing the local discretization error, thus the advantage of improving the accuracy of global outputs intrinsic of adjoint is not an important factor in this case, but can be interesting for future applications. Therefore, the analysis must focus on computational aspects. Even with the interpolation procedures for approximating the finest mesh, the method requires the computation and storage of a fine mesh, one residual evaluation on this fine mesh and finally an adjoint solution on the current mesh. Consequently, the computational cost is still very high, very similar to other discretization error methods. The implementation cost remains as the most important drawback due to the difficulty of obtaining the Jacobian of the system, as the scrape-off layer plasma equations are in general more complex than regular CFD problems, even if one assumes a neutral fluid model such as in this case. Therefore, this adaptation sensor methodology remains out of the scope of this thesis and could be considered for improving global outputs.

\section*{\textit{τ}-estimation}

Unlike other methodologies based on discretization errors, \textit{τ}-estimation exploits the advantages of estimating the truncation error for obtaining an error adaptation sensor. The most interesting one comes from the fact that it does not required multiple converged simulations, but only the evaluation of the residual on other meshes, saving significant computational effort.

The complete methodology of \textit{τ}-estimation employed for mesh adaptation is provided by \cite{14}. Two embedded meshes with a refinement factor between them are necessary for computing the error indicator defined at each cell with node index $i$:

$$I_i^\tau = \frac{|\Omega_{hi}|^\alpha}{1 - \rho^p} |\tau_{hi}^c|,$$ \hspace{1cm} (5.5)

where $\tau_{hi}^c = R_{hc}(U_{hi})$, $\Omega_{hi}$ is the cell volume with an scaling factor $\alpha$, the mesh size ratio is referred as $\rho$ and $p$ the order of accuracy. Observe that it is only required the evaluation of the coarse mesh residual with the fine mesh solution, which obviously implies the storage of a coarse grid every step. Fraysse et al. \cite{13} explain a further improvement in this strategy called “Quasi a-priori mesh adaptation based on \textit{τ}-estimation”, which allows to obtain TE estimates with non-converged solutions. However, this method includes the calculation of Jacobians of the system, which remains out of the scope and can be considered for future plasma applications.
Although this indicator seems very attractive for reducing the discretization errors, the “truncation-error convergence is often misleading for FVD schemes on irregular grids” [9]. As a consequence, an estimation of the true order of accuracy is required for validating the error confidence, which again would be solved by techniques like Richardson extrapolation.

**Richardson extrapolation indicators**

Finally, error sensors based on the well-known Richardson extrapolation (see chapters 3 and 4) allow to estimate actual discretization errors for the scrape-off layer plasma problem. This strategy prevents from having possible convergence issues associated with TE estimation and avoids the prohibitive implementation cost of methods associated with jacobian calculations. On the other hand, the complete three grid Richardson extrapolation implemented in last chapters has too high computational cost for practical adaptive algorithms. However, using two grids to obtain an extrapolated solution by assuming a formal order of accuracy, can be a promising tool for design optimization algorithms, with the drawback of less reliability than the complete version but still with enough accuracy to reduce the relative discretization errors. Therefore, Richardson extrapolation error sensors along with mesh optimization design results as the other candidate for improving the accuracy of the plasma-edge simulations.

5.3 Conclusions

With the premise of not changing the structure of the solver, r-refinement and h-refinement are the mesh adaptation strategies selected for possible discretization error reduction to improve the accuracy of plasma-edge simulations.

The best error sensor candidates for guiding the adaptation process are feature-based error indicators and Richardson-based error indicators. The main advantage of the difference detector is the cheap computational cost as only a single simulation is needed. These type of errors usually work well capturing physical flow phenomena but lack of mathematical foundation as they are not directly related to discretization errors. The application to the plasma-edge bias grid configuration has to be tested. On the other hand, Richardson extrapolation error indicators allow to estimate actual discretization errors preventing from having possible convergence issues associated with TE estimation and avoiding the prohibitive implementation cost of methods associated with jacobian calculations. However, the computational cost is higher than the other methods as multiple grids are required. Therefore, Richardson extrapolation error sensors along with mesh optimization design results as the other candidate for improving the accuracy of the plasma-edge simulations.
Chapter 6

Implementation of feature-based error indicators to the plasma-edge problem

In this chapter, feature-based indicators are implemented into plasma problem in order to test the accuracy of these error sensors to guide a possible h-refinement algorithm. The first section corresponds to the application of the classical approach of the difference detector. The adaptation of this method to structured grids is achieved in later sections along with the comparison with actual discretization error estimates.

6.1 Classical approach

The difference detector is a feature-based error indicator that can be defined as the undivided difference between the solution at a cell and the solution at its adjacent neighbor cells. This parameter allows to store the change of the solution from one cell to the next one, giving some insight about how the mesh captures the solution profiles in each coordinate direction.

Therefore, six difference detectors are defined at each cell indexed by $i$:

- Four face detectors: $C_{f-north}^i$, $C_{f-east}^i$, $C_{f-south}^i$ and $C_{f-west}^i$, which are calculated with the expression $C_{f-j}^i = |u(x_i) - u(x_j)|$ with $j = \{north, east, west, south\}$. After normalization, these indicators help the algorithm to decide whether to keep or remove each face in order to coarse the cell. If the indicator is below some predefined threshold, the face is flagged to be removed.

- Two cell detectors: $C_X^i$ and $C_Y^i$, obtained as the average of the two face detectors that belong to faces perpendicular to the coordinate direction considered (e.g. $C_X^i = \frac{C_{f-east}^i + C_{f-west}^i}{2}$). On the other hand, these parameters allow to decide whether to make a split or not perpendicular to the coordinate
6. Implementation of feature-based error indicators to the plasma-edge problem

The implementation of these difference detectors to plasma-edge problem with a grid of 70x20 cells with exponential refinement toward the targets (bias grid case) was performed to the ion density and ion temperature. The following figures illustrate an example of the results: the Cx indicator for the ion density and the Cy indicator for the ion temperature. Observe that both indicators capture the changes along each direction in the solution profiles: the highest Cx ion density sensors are located at the targets, especially in the SOL, whereas the the Cy ion temperature sensors describe accurately how the temperature decreases in the radial direction from the core towards the SOL, providing information about what regions should be refined or coarsed.

6.2 Approach for structured grids

The classical approach of splitting or coarsening cell by cell based on feature indicators has been successfully tested for scrape-off layer plasmas in [19]. This strategy generally is only possible for unstructured grids, in which the storage of the resulting hanging nodes - consequence of the refinement - is achieved naturally due to the type of data structure. In [19], the B2 code is adapted to support unstructured grids so that the feature indicators can be used for h-refinement, yielding good results in the mesh adaptation.

However, the Matlab plasma code studied in this thesis employs structured grids that would require the adaptation of the solver, including all the discretization schemes and data structure, which is not intended for this work. Therefore, different approaches that respect the current data structure have to be tested. One simple procedure to avoid hanging nodes is by making decisions on splitting or coarsening rows or columns instead of single cells. There are two type of approaches for obtaining error indicators representative of entire rows and columns:

1. **Average of indicators along a coordinate direction.** This strategy provides radial-averaged indicators for each column or poloidal-averaged indicators...
6.3. Comparison with discretization error estimates

![Graph](image)

**Figure 6.2:** Results for the Cx error indicator of ion density (upper figure) and Cy error indicator of ion temperature (lower figure).

for each row. Consequently, the total error would be reduced but the average could mask regions needed to be refined such that the local error may not necessarily be reduced.

2. **Maximum of indicators along a coordinate direction.** Poloidal and radial indicators are obtained with the maximum value of each row or column respectively. This allows to reduce the local errors, but it could lead to over-refinement as only a single cell above the threshold would flag the entire row or column to be refined.

To continue with the examples showed in last section, the results for Cx radial-averaged indicators of the ion density and Cy poloidal maximum indicators of the ion temperature are shown in figures 6.3 and 6.4. In these examples, an action threshold was set. All row or column indicators above it were marked in red to be splitted.

6.3 Comparison with discretization error estimates

Up to this point, there is no actual evidence that the difference indicator provides a good measure of the discretization error. In order to test the accuracy of these structured grid approach indicators, a comparison of each of the six cell detectors obtained by the two approaches (average and maximum) were compared to the
6. Implementation of feature-based error indicators to the plasma-edge problem

Figure 6.3: Cy poloidal maximum indicators of the ion temperature before and after being flagged to be refined (upper and lower figures respectively).

Figure 6.4: Cx radial-averaged error indicators of the ion density before and after being flagged to be refined (upper and lower figures respectively).
profiles of discretization error estimated by Richardson extrapolation, which have been normalized and adapted following the same approaches explained in last section. The results showed that, for certain cases the indicators captured accurately the regions with highest discretization errors, whereas the same indicators on other cases did not locate at all these regions. Therefore, the accuracy of the indicators depends on each particular case and can not be generalized for any application. An example of these results is provided, in which the Cy indicator (poloidal maximum approach) achieves high precision for the ion temperature (upper figure) but completely fails for the ion density (lower figure).

Figure 6.5: Comparison of Cy indicator and normalized discretization error estimated by RE, both calculated following the poloidal maximum approach, for the ion temperature (upper figure) and ion density (lower figure).

6.4 Conclusions

In order to avoid hanging nodes typically obtained with h-refinement strategies applied cell by cell, an adaptation with two different approaches of the classical undivided difference detector to structured grids is proposed. The first approach consists on averaging the indicators along a coordinate direction, whilst the second one employs the maximum value of an entire row or column. These indicators are used along with thresholds to decide whether to split or coarse an entire row or column. The application to the plasma-edge model showed that just for certain
6. IMPLEMENTATION OF FEATURE-BASED ERROR INDICATORS TO THE PLASMA-EDGE PROBLEM

cases the indicators captured accurately the regions with highest discretization errors. Therefore, the accuracy of the indicators depends on each particular case and cannot be generalized for all the state variables in other grid configurations. For this case, these feature error sensors do not provide sufficient accuracy for driving a mesh adaptation process to reduce the discretization errors.
Chapter 7

Mesh optimization using Richardson extrapolation as adaptive error sensor

This final chapter studies the application of PDE-constrained design optimization to the plasma-edge problem in order to obtain the optimal grid configuration that reduces the local discretization error of a desired state variable. The error sensor that helps to build a suitable cost functional will be obtained by Richardson extrapolation.

7.1 PDE-constrained optimization

PDE-constrained optimization problems are found in the framework of large-scale optimization. Within this category, one can distinguish two types depending on whether the partial differential equations are discretized before solving the optimization (Discretize-Optimize approach) or a continuum optimization problem is solved first to obtain a set of equations to discretize (Optimize-Discretize approach) [17]. PDE optimization problems have been carefully studied in recent years by numerous authors in very different engineering areas. Of particular interest are design shape optimization problems [15], which focus on attaining optimal geometry (or mesh configuration) for improving the accuracy of a certain global output e.g. aerodynamic coefficients, by minimizing an objective functional. This objective functional can be formulated aiming discretization error reduction [16]. Among the research in nuclear fusion, important works are provided by Dekeyser et al [7][8], in which shape optimization applied to divertor target shape has been introduced, whereas Blommaert et al [3] have provided a complete automated approach for designing an optimal divertor magnetic configuration aiming the maximum spread of heat load over the divertor target area.
7. Mesh optimization using Richardson extrapolation as adaptive error sensor

7.2 Formulation of the plasma-edge mesh optimization problem

The general formulation of the PDE-constrained design optimization problem applied to the plasma-edge transport model is provided by Blommaert et al [3]. Thus, the optimization problem can be written as:

\[
\begin{align*}
\text{minimize} & \quad \Gamma(\varphi, q) \\
\text{subject to} & \quad c(\varphi, q) = 0 \\
& \quad h_i(\varphi, q) \leq 0, \quad i = 1, \ldots, m.
\end{align*}
\] (7.1)

where \( \Gamma(\varphi, q) \) is the cost functional evaluating the discretization error of a desired state variable (e.g. ion density discretization error). \( c \) represents the magnetic field calculation, the grid generation aligned with the magnetic field lines and the plasma-edge equations that simulate the plasma state. The design variables \( \varphi \) correspond to mesh parameters that generate the grid configuration, which have to satisfy some design constrains \( h_i \) as well as belong to set of feasible values \( \Phi_{ad} \). The state variables \( q \) can be eliminated from the optimization problem by using equations \( c = 0 \), yielding a reduced optimization problem of the form:

\[
\begin{align*}
\text{minimize} & \quad \hat{\Gamma}(\varphi) \\
\text{subject to} & \quad \hat{h}_i(\varphi) \leq 0, \quad i = 1, \ldots, m.
\end{align*}
\] (7.2)

where \( \hat{\Gamma}(\varphi) = \Gamma(\varphi, q(\varphi)) \) represents the reduced cost functional and \( \hat{h}_i \) the reduced design constrains. In the reduced problem, state variables do not have to be taken into account as control parameters as the plasma-edge simulation is treated as a black-box solver, thus resulting in an problem with significant less dimensionality. Reduced optimization problems are generally solved by sequential quadratic programming (SQP), which will be addressed in section 7.2.2.

7.2.1 The cost functional

The grid configuration to be optimized is referred as the “bias grid by zones” with 140x40 cells, which consist of a mesh divided in three different zones separated by the cuts in the slab domain (left and right divertors legs and central zones involving part of SOL and core regions). In each zone, an exponential poloidal refinement starting from a central region toward the boundaries is performed. The exponential refinement parameter, so-called in this work “bias factor”, is the control variable used for the mesh parametrization of the three zones (See chapter 4).

The aim of the mesh optimization is to find a grid defined by the optimal bias factor that minimizes the relative local discretization errors of a state variable, in this case, the ion density. Mesh optimization usually pursues the equidistribution of error over the domain by employing global norms of the discretization errors. As predicted in chapter 4, the highest discretization errors of the ion density are located...
7.2. Formulation of the plasma-edge mesh optimization problem

at the targets mainly due to the extreme gradients that occur in this narrow region. Therefore, a suitable objective functional have to be formulated, which can be also used for other state variables. Before discussing the different options, a general expression for the reduced cost functional is provided:

\[ \hat{\Gamma}(b) = \frac{1}{2\kappa} \left( \frac{U_{\text{ref}} - U_h}{U_{\text{ref}}} \right)^2_{L_2}, \]  

(7.3)

which corresponds to a sum of square relative discretization errors ($L_2$ norm) where $U_{\text{reference}}$ is the reference solution for the ion density, $U_h$ is the solution on the current mesh and $\kappa$ refers to a normalization factor.

In order to reduce the local relative errors at the targets, it is important that the errors calculated after every optimization iteration are compared at the same physical locations in the domain. Since the nodes move along the domain with every update of the bias factor, the discretization errors are estimated at different locations. To solve this problem, an intermediate step is introduced that interpolates the estimated errors from the current mesh to an equidistant mesh that is kept constant in the whole optimization process. Additionally, the cost functional becomes more sensitive to changes of the bias factor if a weighting procedure is applied such that the target region provides the greatest contribution to the total sum of square errors. Instead of defining node weights at every region, an equivalent alternative is to include a higher number of nodes in the divertor legs, resulting in three equidistant meshes, each with a number of poloidal cells proportional to cells employed in each zone of the original mesh (e.g. 50 poloidal cells at the divertor legs in comparison to the 40 cells of the central region). The radial cells are constant for every zone. Finally, the total number of equidistant nodes is employed as normalization factor for scaling the objective functional.

The reference solution that provides a discretization error sensor for guiding the adaptation process is obtained by Richardson extrapolation. Two possible options for the cost function are then defined:

**Reference solution that excludes dependance on the bias factor**

In the first optimization iteration, the reference solution $U_{RE}$ is obtained by employing complete Richardson extrapolation with the current mesh as fine mesh, and two additional auxiliary coarser meshes. The observed order of accuracy is treated as an unknown that is estimated point-wise. Therefore, the extrapolated solution on the original mesh with bias factor $b_{\text{ref}}$ is kept constant through the optimization process as the control parameter is not included in the reference. This objective function is formally expressed as:

\[ \hat{\Gamma}(b) = \frac{1}{2\kappa} \left( \frac{U_{RE} - U_h(b)}{U_{RE}} \right)^2_{L_2}. \]  

(7.4)

This is the less CPU demanding option amongst all, as only the first iteration requires multiple state solutions on different meshes. Conversely, the size of the smallest cell of the original reference mesh sets the limit for refinement as the
Mesh optimization using Richardson extrapolation as adaptive error sensor

Resolution in that region cannot be outperformed by the adapted mesh. Consequently, if the reference mesh consist of a bias grid configuration with bias factor $b_{ref}$, the adapted mesh - with same grid parametrization but with different initial bias factor $b_0$ - will tend to the reference value, becoming a fitting problem. Therefore, this strategy only yields successful results if the reference mesh has a uniform cell distribution with no relation to the adapted grid. Since the aim of the optimization problem is to improve the accuracy at the targets, a uniformly refined mesh with sufficient resolution becomes too CPU demanding to serve as reference in practical applications.

Reference solution that includes dependance on the bias factor

On the other hand, if the dependance on the control parameter is included in the extrapolated solution $U_{RE}(b)$, the reduction of discretization error is achieved automatically for any grid configuration by the optimization problem, providing that the objective function is sufficiently convex or a regularization term must be included. The objective functional that includes the bias factor is

$$\hat{\Gamma}(b) = \frac{1}{2\kappa} \left\| \frac{U_{RE}(b) - U_h(b)}{U_{RE}(b)} \right\|^2_{L_2}.$$ (7.5)

There are two possibilities for obtaining the Richardson extrapolated solution:

1. Using three grids in every optimization iteration (current fine mesh and two auxiliary coarser meshes) for calculating the observed order of accuracy. This is the most reliable option, but it is completely impractical as it is extremely CPU demanding even though only one control parameter is considered. Multiple control variables makes the problem even more demanding because of the additional gradient calculations. Line search strategies for determining optimal step size make this option unreasonable as well.

2. Using two grids in every optimization iteration (current fine mesh and one auxiliary coarser mesh) and assuming the formal order of accuracy as constant. This option is less reliable than the last option in terms of error prediction, but still sufficiently accurate to provide a good estimation of discretization error distribution in comparison to other adaptive error sensors. In addition, the savings in computational effort respect to the three grid case are very important. Therefore, it is the cost functional selected for the optimization of the bias grid.

7.2.2 Optimization algorithms

Reduced optimal problems are generally solved by sequential quadratic programming, a strategy that subdivides the original problem in local quadratic Taylor approximations of the reduced objective functional and reduced constrains at every iteration $[3][21]$. The Hessian is approximated by different methods e.g. BFGS algorithm, which only uses information of gradients on the past and current iterations to estimate the curvature. In order to find an optimal step size after obtaining the search direction from a quadratic subproblem, inexact line search is normally
7.3. Mapping of cost function for bias grid configuration

performed to satisfy Armijo’s condition with backtracking that ensures that the steps are short enough to get sufficient decrease and long enough to not get stuck [21].

However, at certain cases in which design contrains \( h_i \) are not necessary, but only ensure that the control variables stay in the feasible set (direct contrains), the optimization problem is simplified into unconstrained optimization, solved directly by Newton type methods. As happens in this particular case, the bias factor is the only control variable that must stay within some limits for the plasma simulations to work properly (0.6 ≤ \( b \) ≤ 1). Two strategies for approximating the Hessian will be used for the optimization of the bias grid: (i) the steepest descent method along with a conservative relaxation factor for the gradient (\( \alpha = 5 \cdot 10^{-4} \)) and (ii) BFGS with line search satisfying Wolfe conditions.

7.2.3 Gradient calculation

The gradients of the quadratic cost functional at every step are calculated using finite differences. Because of the numerical noise [5], the cost function may present small oscillations that would make the gradient estimation to fail if the perturbation is very small (10\(^{-4}\)). Therefore, the size of the perturbation can be increased until the behavior of cost functional is accurately captured. In this case, since the bias factor can vary from 0.6 to 1, a suitable perturbation is 0.02, that prevents from problems that arise from oscillations of numerical noise or even other possible local minima. If the cost functional shows important non-convex behavior, regularization terms or other more advanced techniques may be applied [2][5].

Finite differences or any form of forward differentiation for calculating the derivatives implies \( n_{\phi} + 1 \) evaluations of the objective functional at every step. In this simple case \( n_{\phi} = 1 \), but if one wishes to include a higher number of mesh parameters like cell width for each coordinate direction, the gradient calculations become extremely computationally demanding. In this sense, a better approach is necessary. Adjoint methodology provides the tool for calculating the gradients of the cost functional with respect to a high number of control parameters at a cheaper cost, as the gradient calculation is achieved by a matrix inversion of the adjoint linear system [16]. The main disadvantage is the formulation of the discrete adjoint system, which involves the complex analytical derivation of the discrete Jacobians, especially in plasma transport equations. Extensive research in adjoint approach to design can be found in [7][18][15].

7.3 Mapping of cost function for bias grid configuration

Before the application of the optimization to bias grid configuration, a mapping of the cost functional is performed by calculating discrete points from \( b = 0.6 \) to \( b = 1 \) every 0.025 units. At each point, a solution extrapolated from a fine mesh with bias factor \( b \) and a coarse mesh embedded is required. This plot will be the reference to confirm if the optimization algorithm reaches the actual global minimum, which is
7. Mesh optimization using Richardson extrapolation as adaptive error sensor

placed approximately at \( b = 0.825 \). It has been tested that fully converged solutions (tolerance of \( 10^{-8} \)) are not necessary to obtain this cost functional. Employing tolerances of order \( 10^{-1} \) are sufficient for the algorithm. As a consequence, significant computational time will be saved.

![Graph showing objective functional value as a function of the bias factor](image)

Figure 7.1: Mapping of objective functional value as a function of the bias factor.

7.4 Results

The change of the control variable (bias factor) and cost functional are given as a function of the optimization iterations in figure 7.2. As it can be observed, the optimization starts from an initial guess \( b_0 = 0.95 \) and evolves until convergence at the optimal value \( b_{\text{opt}} = 0.8257 \). Regarding the steepest descent method, the optimization process takes 17 iterations to converge (\( \nabla b \hat{\Gamma} \approx 0 \)). The cost functional drops quickly in the first iterations but then the convergence becomes slower, which corresponds to the expected behavior of a steepest descent method without line search (the step size decreases proportional to gradient). Despite the high number of optimization iterations, the total computational time spent is equivalent to just four fully-converged plasma state simulations on the fine mesh (in addition to the auxiliary coarser simulations), thanks to the tolerance set to \( 10^{-1} \). The BFGS algorithm with line search, outperforms the steepest descent method in terms of convergence speed, as the optimum is reached in just 5 iterations. This more advanced strategy is more suitable when one wishes to optimize cases of more complexity, in which information of the cost functional is not easily available and a more automated approach is required.

The optimization has provided an optimal mesh configuration that reduces the relative discretization error. To verify the error reduction, the relative discretization
errors for the ion density are plotted for two cases: (i) The initial mesh with $b_0 = 0.95$ and (ii) final mesh with $b_{opt} = 0.8257$. As figure 7.3 shows, the optimization has achieved a relative error reduction from 15% to 4.5% of maximum errors.

Figure 7.2: Change of the control variable (bias factor) and cost functional are given as a function of the optimization iterations for (i) the steepest descent method and (ii) BFGS with line search.

7.5 Conclusions

A mesh optimization method aiming relative discretization error reduction has been applied to the plasma-edge model. The method implemented in Matlab follows the methodology of PDE-contrained design optimization. First, a cost functional based on Richardson extrapolation was formulated including interpolation and weighting procedures which help to estimate the relative discretization errors at the same physical locations. This design allows to compare the relative errors after every iteration. The error sensors are obtained by applying Richardson extrapolation to the current mesh with the help of an auxiliary coarser mesh at every optimization step. The test case was an optimization of a bias grid configuration with the goal of
7. Mesh optimization using Richardson extrapolation as adaptive error sensor reducing the discretization error of the ion density. This type of mesh is characterized by an exponential refinement toward the boundaries defined by the control parameter so-called bias factor. Two optimization strategies to approximate the Hessian of the objective function were tested: (i) the steepest descent method without line search and (ii) BFGS with line search satisfying Wolfe conditions. After the application, the control parameter evolved from an initial guess of $b_0 = 0.95$ to an optimal value $b_{opt} = 0.8257$, achieving a relative discretization error reduction of 10% between the maximum values of both configurations (from 15% to 5%).

Figure 7.3: Reduction of relative discretization error achieved by the optimization. The errors shown belong to the initial mesh with $b_0 = 0.95$ (above) and final mesh with $b_{opt} = 0.8257$ (below).
Chapter 8

General conclusions

In the first part of this work, different discretization error estimation methodologies are collected from the field of computational fluid dynamics to study their applicability to a plasma-edge model. The basic points for the comparison of these techniques are the accuracy, computational cost and implementation cost. It was found that Richardson extrapolation is the most suitable discretization error strategy as it combines a low implementation cost, compared to other code-intrusive methods (e.g. DETE and p-refinement) or those that require the calculation of complex jacobians (e.g. adjoint methodology), at a similar expense of computational effort. Additionally, it provides a reliability assessment on the confidence of error estimates as an intrinsic step of the extrapolation procedure.

Richardson Extrapolation methodology is thus applied to the plasma-edge problem in order to estimate the distribution of discretization error of the ion density and ion temperature over the 2D slab case domain. The domain was discretized with two types of meshes: (i) a “biased grid” with 280x80 cells, with exponential refinement towards the divertor targets and (ii) a “bezier grid” with 720x40 cells, comprised of two zones with different level of equidistant refinement smoothly joined by a bezier curve transition. The method employed in the algorithm to rebuild solutions at the coarse grid points was an integration procedure. The analysis of the observed order of accuracy for each variable in the bias grid case revealed that several regions in the domain presented slow convergence with refinement or even non-asymptotic behavior, providing low reliability of the error estimates on these zones. It was suspected that the low mesh quality of the bias grid (very high aspect ratios) was responsible of this behaviors. For this matter, the bezier grid configuration was tested resulting in a great overall improvement of the observed order. However, there were still some regions with slow convergence and asymptotic behavior, that may be explained with insufficient refinement or even caused by local characteristics of the problem itself, such as the oscillatory behavior that can occur when combining mixed-order schemes in a convection-diffusion equation. In order to fix the reliability problem associated with slow convergence and non-asymptotic behavior, the discretization errors were converted into uncertainty errors by the GCI method with recommendations of Oberkampf and Roy. After applying it to the bias grid and bezier grid cases, the
distribution of GCI-OR discretization error was finally obtained for each plasma state variable at each case. Regarding the ion density of the bias grid configuration, the highest relative errors were concentrated at the divertor targets in the scrape-off layer, yielding values around 5%. For the ion temperature, maximum relative errors (8.7% - 10.4%) were located near the X-point. On the other hand, the bezier grid results showed a similar distribution of error but with inadmissible errors confirming that the improvement in the order of accuracy does not justify the selection of this mesh because of its poor mesh resolution for the plasma-edge problem.

In the second stage of the thesis, the goal of finding a mesh adaptation method for reducing the discretization errors of the plasma state variables is tackled. First, it was concluded that the best error sensor candidates for guiding the adaptation process are feature-based error indicators and Richardson-based error indicators.

In order to avoid hanging nodes typically obtained with h-refinement strategies applied cell by cell, an adaptation with two different approaches of the classical undivided difference detector to structured grids is proposed. The first approach consists on averaging the indicators along a coordinate direction, whilst the second one employs the maximum value of an entire row or column. The application to the plasma-edge model showed that just for certain cases the indicators captured accurately the regions with highest discretization errors. Therefore, the accuracy of the indicators depends on each particular case and can not be generalized for all the state variables in other grid configurations. For this case, these feature error sensors do not provide sufficient accuracy for driving a mesh adaptation process to reduce the discretization errors.

The final contribution of this work is the development of a mesh optimization method aiming relative discretization error reduction applied to the plasma-edge model. The method, implemented in Matlab, follows the methodology of PDE-constrained design optimization. First, a cost functional based on Richardson extrapolation was formulated including interpolation and weighting procedures which help to estimate the relative discretization errors at the same physical locations. This design allows to compare the relative errors after every iteration. The error sensors are obtained by applying Richardson extrapolation to the current mesh with the help of an auxiliary coarser mesh at every optimization step. The test case was an optimization of a bias grid configuration with the goal of reducing the discretization error of the ion density. Two optimization strategies to approximate the Hessian of the objective function were tested: (i) the steepest descent method without line search and (ii) BFGS with line search satisfying Wolfe conditions. After the application, the control parameter evolved from an initial guess of $b_0 = 0.95$ to an optimal value $b_{opt} = 0.8257$, achieving a relative discretization error reduction of 10% between the maximum values of both configurations (from 15% to 5%).

For future work, these techniques could be extended to a full plasma-edge code such as B2-Eirene. Furthermore it would be desirable to study the feasibility of implementing a discrete adjoint approach for the gradient calculations of the mesh optimization algorithm, since it would allow to increase significantly the number of mesh control parameters (e.g. width of each cell) with an affordable computational cost.
Chapter 9

Planification and budget

9.1 Planification

The development of the project is very linear since it corresponds to a typical research project in which every phase requires its previous phase to be completely finished to be able to start.

The time scope of the project is of 1 year and 45 days, starting from the 26th of August 2015. The project is divided into five different phases, as it can be observed in the Gantt diagram (figure 9.2):

1. The planification of the project was agreed in the final week of August 2015 in a meeting with the Promote Martine Baelmans and mentors Maarten Blommaert and Niels Horsten. A roadmap was give including some deliverables that have to be provided at meetings. Additionally, it was arranged a meeting for every month approximately with the promoter to supervise the progress of the project. On the other hand, meetings with mentors were set for every Thursday at 10:30.

2. The literature survey is planned to start for the 1st of September 2015, with a time duration of 1 month. This stage helps to get familiar with nuclear fusion physics and its context. This phase includes introductory courses about plasma-edge physics and tokamak devices.

3. The study of discretization error estimators. The real research commences with the tackling of the first goal of the project, which aims to find a suitable discretization estimator for the plasma-edge problem. Therefore, an intensive research in the field of computational physics is require to be able to collect the most significant methods that might be possible to apply for the problem studied. Additionally, a comparative analysis has to be performed to conclude with the most suitable methodology to apply in the next step. After the feasibility study, the implementation of the selected method takes place, which in principle cover the majority of the time scope of this phase, for the difficulty of implementation as well as for possible unexpected events that may slow down the progress.
4. **The mesh adaptation phase.** The next stage of the project covers the objective of improving the numerical accuracy of the current meshes by developing an adaptation algorithm. In this stage an optimization approach is desired to be able to automatize the mesh generation process, which requires of through literature review from the field of CFD to be able to extend it to the Matlab code. For this reason, this phase plays a critical role in the time scope of the project and thus, the final date has been revised during the project since it was not clear from the beginning if the optimization phase would be completed for June, as it was expected to be very difficult to implement and the computer simulations have an enormous computational cost.

5. The final phase is the **documentation**, in which the written documents must be delivered before deadlines at both Universities (KU Leuven and UPM-ETSII). The oral presentations are set for the 30th of August 2016 at KU Leuven and for the 14th of October 2016 at UPM-ETSII.

With the goal of helping to identify easier the participants of the project, a decomposition of the project scope is given in figure 9.1. The project is held by the KU Leuven and Universidad Politécnica de Madrid. Tasks comprehending research, development and documentation of this project are accounted to Javier Riverola. Supervision and guidance tasks are subdivided in promotion and monitoring duties, whose responsible are Martine Baelmans (KU Leuven) and Gonzalo Jiménez. Mentoring and weekly supervision is performed by engineers Maarten Blommaert and Niels Horsten of the Department of Mechanical Engineering at the Faculty of Engineering Science (KU Leuven)

![Figure 9.1: Decomposition of the project scope.](image-url)
9.2 Budget

In this section, all resources required for the successful completion of the project scope are presented as well as the cost and time spent. As a research University project using mainly homemade simulation codes, only a few physical resources are needed:

- Personal and auxiliary computers with four cores per unit, adding a total amount of CPU power of 12 cores. The total amount of CPU time spent is estimated to be of 900 working hours plus the simulation time of 1.5 months approximately, accounting for all simulations (optimization cycles spend around one week to obtain converged solutions). The estimated cost of CPU time is 0.07 euros/core hour.

- Matlab license costs 1200 euros for the duration of the project.

The human resources are compound of the participants of the project at Universities KU Leuven and UPM-ETSII, which have been involved in different areas of the project as is it described in figure 9.1. The estimated cost for each part of the project scope is calculated from the cost per hour for each of the members involved using averaged salaries for each position as reference. The simplicity of the project scope allows to summarize the final budget of the project in a simple table, which accounts for a total cost of 14857.2 euros:

<table>
<thead>
<tr>
<th>Responsible</th>
<th>Time (h)</th>
<th>Cost (euros)</th>
</tr>
</thead>
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<td>Research and documentation</td>
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<td></td>
</tr>
<tr>
<td>J. Riverola</td>
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<td>11250</td>
</tr>
<tr>
<td>Supervision</td>
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<td></td>
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<td>M. Baelmans</td>
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<td>875</td>
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<td>G. Jimenez</td>
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<tr>
<td>Mentoring</td>
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<td>M. Blommaert</td>
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<tr>
<td>N. Horsten</td>
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</tr>
<tr>
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</tr>
<tr>
<td>Matlab License</td>
<td>1200</td>
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<tr>
<td>Total</td>
<td>2065</td>
<td>14857.2</td>
</tr>
</tbody>
</table>

Table 9.1: Budget of the project.
9. Planification and budget

Figure 9.2: Gantt diagram.
Chapter 10

Social responsibility

Engineers and scientists working on current research and development projects in the field of nuclear fusion technology are the takers of the torch in the race of mankind to obtain a clean and virtually inexhaustible source of energy. Thus, they are followers of an effort started decades ago by some of the clearest minds emanating from the international scientific community, which entails a responsibility to understand, improve, and pass that knowledge correctly.

The design, construction and commissioning of a Tokamak reactor involves enormous complexity and it is a scientific and technological challenge of such magnitude that is near the limit of our technological capacity. The closer the target is the more important is to ensure the proper use of technical and human resources invested by our society in what will be a heritage of humanity achievement. In that sense, the virtues that are part of the engineering code of ethics are key to further progress towards the goal of building the future reactor. The generation of energy in an environmentally friendly way, in a safe facility for operators and the general public, which is one of the essential motivations of nuclear fusion technology, has to be not only an aspiration, but an indispensable objective.

Researchers conducted in simulation and optimization of Tokomaks, framework in which this project is located, are part of a professional group in which ethical attitudes such as objectivity in judgments and assessments, transparency and traceability in the reports, sincerity on results, respect for intellectual property, commitment to legislation in the nuclear field, fair competition, and build a foundation of trust are essential. The professional involved in such developments should always engage in their particular environment with these principles of action consciously, and generally give priority to those issues of respect for the environment and public safety above other also important aspects, such as economic or political. Therefore, due to the nature and scope of their professional activity, engineers and researchers in nuclear fusion are the subject of a high ethical and social responsibility.
Bibliography


Bibliography


