High Order Time-Accurate Partitioned Simulation of Unsteady Conjugate Heat Transfer

Analysis and Application of Implicit Runge-Kutta Time Integration Schemes

Vahid Kazemi Kamyab
High Order Time-Accurate Partitioned Simulation of Unsteady Conjugate Heat Transfer

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Vahid KAZEMI KAMYAB

(Master of Mechanical Engineering,
The City College of the City University of New York, U.S.)
egenoren te Tehran, Iran.
Dit proefschrift is goedgekeurd door de promotor:

Prof. dr. ir. drs. H. Bijl

Copromotor:

Dr. ir. A.H. van Zuijlen

Samenstelling promotiecommissie:

Rector Magnificus
Prof. dr. ir. drs. H. Bijl
Dr. ir. A.H. van Zuijlen
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Summary

Thermal interaction of flows and structures, also referred to as conjugate heat transfer, arises in many engineering applications, where heat conduction in a solid is coupled to heat convection in an adjacent fluid. Examples include geothermal heat exchanger systems, cooling of micro-electronic chips, interstitial thermal therapy, and immersion lithography. Conjugate heat transfer (CHT) encountered in many of these engineering applications is unsteady, and accurate determination of the transients is essential in enhancing efficiency and/or safety of designs. However, time-accurate computations of CHT can be computationally expensive. Furthermore, given the multi-physics nature of many engineering problems, resolution of other coupled phenomena, in addition to CHT, may also be of interest.

This thesis aims at developing a flexible and efficient numerical procedure for solving unsteady (transient) conjugate heat transfer. High order implicit time integration schemes are considered in order to reduce the computational work of solving time-accurate CHT problems. For flexibility, the partitioned method is adopted for solving the coupled problem. Depending on the strength of the thermal interaction between the subdomains, it is in general computationally more efficient to select either a loosely-coupled or strongly-coupled algorithm. The ratio of the thermal effusivities of the coupled domains denoted by \( \sigma \) is used as a measure of the strength of the thermal interaction: when \( \sigma \ll 1 \), the strength of the interaction is weak, and as \( \sigma \to 1 \) the strength of the interaction increases.

For strongly coupled problems, a strongly-coupled solution algorithm is presented where high order explicit first stage singly diagonally implicit Runge-Kutta (ESDIRK) schemes are used for time integration. For Dirichlet-Neumann conditions at the interface, stability and rate of convergence of (Gauss-Seidel) subiterations at each stage of the ESDIRK schemes are analyzed analytically. Based on the analysis, the domain with the higher effusivity is assigned the Neumann condition and the one with the lower effusivity the Dirichlet condition. Furthermore, the interface iterations converge with a rate approximately given by \( \sigma \). The results obtained by solving a CHT test-case, show good agreement with the performed analytical stability analysis.
For weakly coupled problems, a loosely-coupled solution algorithm is presented in which a family of high order implicit-explicit (IMEX) Runge-Kutta schemes are used for time integration. The IMEX schemes consist of the ESDIRK schemes for advancing the solution in time within each subdomain, and equal order and number of stages explicit Runge-Kutta (ERK) schemes for explicit integration of part of the coupling terms.

Given similarities between the second stage of the loosely-coupled IMEX schemes and the predictor-corrector Crank-Nicolson scheme, first analytical accuracy and stability analyses are performed for the latter scheme. Next, accuracy and stability of the loosely-coupled IMEX schemes are investigated numerically, using the analytical results of the Crank-Nicolson scheme as reference. By considering a CHT test-case, temporal order preservation of the coupling algorithm (without subiterating) is demonstrated. From the stability investigation it is concluded that when $\sigma \ll 1$, the loosely-coupled IMEX schemes remain stable to large Fourier numbers $d_m$, indicating that time-step size is restricted by accuracy rather than stability.

For both the loosely and strongly coupled solution algorithms, by respectively considering a weakly coupled and a strongly coupled CHT test-case, the work-precision character of the high order time integration schemes and the commonly used second order implicit schemes are compared over a range of accuracy requirements. For time-accurate solutions, the high order schemes are observed to be computationally more efficient relative to the second order schemes. The computational gain is higher as smaller tolerances are sought.

Another topic studied in this thesis is the application of high order ESDIRK schemes to cell-centered collocated finite volume discretization of unsteady incompressible Navier-Stokes equations. In particular, a face-velocity interpolation procedure (Rhie-Chow) which preserves the temporal design order of the multi-stage ESDIRK schemes is introduced. In addition, the influence of iterative errors on temporal order is minimized by using an iterative time advancing algorithm. The results of numerical examples demonstrate the temporal order preservation of the algorithm.
Samenvatting

Thermische interactie tussen vaste en vloeistoffen, ook wel aangeduid met conjugaat warmteoverdracht, bestaat in veel technische toepassingen, waarbij warmteconduktie in vaste wanden gekoppeld is met warmte convectie in een aangrenzende vloeistof. Voorbeelden hiervan zijn geothermische warmtewisselvelden, koeling van micro-chips, interstitiële thermische therapie en immersie lithografie.

Dit proefschrift is gericht op het ontwikkelen van een flexibel en efficiënt numeriek algoritme voor het simuleren van instationaire (voorbijschijnende) thermische interactie van vloeistoffen en vaste stoffen, ofwel conjugaat warmteoverdracht (CHT). Hoge orde impliciete tijdsintegratie methodes worden overwogen teneinde het rekenwerk voor het nauwkeurig simuleren van CHT in de tijd te verminderen. Voor flexibiliteit, wordt een gepartitioneerde aanpak gebruikt voor het oplossen van het gekoppelde probleem. Afhankelijk van de sterkte van de thermische koppeling, is ofwel een zwak dan wel sterk gekoppeld algoritme het meest efficiënt. De ratio van de thermische effusiviteit van de gekoppelde domeinen $\sigma$ wordt gebruikt als een maat voor de sterkte van de thermische koppeling: wanneer $\sigma \ll 1$ is de sterkte van de koppeling zwak en als $\sigma \rightarrow 1$ neemt de sterkte van de koppeling toe.

Voor thermisch sterk gekoppelde problemen is een sterk gekoppeld oplossingsalgoritme gepresenteerd waarin de hoge orde, expliciete eerste trap, enkelwaardige diagonaal-impliciete Runge-Kutta (ESDIRK) methodes worden gebruikt voor tijdsintegratie. De stabiliteit en convergentie snelheid van (Gauss-Seidel) subiteraties met Dirichlet-Neumann randvoorwaarden op de interface zijn analytisch geanalyseerd voor elke trap van de ESDIRK schema’s. De analyse toont aan dat het domein met de hogere effusiviteit de Neumann randvoorwaarde behoort te hebben en het domein met de lagere effusiviteit de Dirichlet conditie.

Voor thermisch zwak gekoppelde problemen is een zwak gekoppeld algoritme gepresenteerd, waarin een familie van hoge orde impliciete-expliciete (IMEX) Runge-Kutta schema’s wordt gebruikt voor tijdsintegratie. Het IMEX algoritme bestaat uit een ESDIRK schema voor de tijdsintegratie binnen elk subdomein en een expliciet Runge-Kutta (ERK) schema van gelijke orde en met het zelfde aantal trappen voor het expliciet integreren van een deel van de koppelingstermen.
Gezien de gelijkenis tussen de tweede trap van het IMEX schema en het predictor-corrector Crank-Nicolson schema, is voor het laatstgenoemde schema een analytische nauwkeurigheids- en stabiliteitsanalyse uitgevoerd. Vervolgens zijn nauwkeurigheid en stabiliteit van de IMEX schema’s numeriek onderzocht, waarbij de analyseresultaten van het Crank-Nicolson schema als referentie dienden. Voor een CHT testprobleem, wordt het orde behoud van de hoge orde IMEX schema’s (zonder subiteraties) aangetoond. Uit het stabiliteitsonderzoek wordt geconcludeerd dat voor $\sigma \ll 1$ de IMEX schema’s stabiel blijven voor grote Fourier getallen $d_m$, wat aangeeft dat de tijdstap grootte wordt beperkt door nauwkeurigheid in plaats van stabiliteit.

De hoeveelheid rekenwerk voor een bepaalde, gewenste nauwkeurigheid is bepaald voor gepartitioneerde algoritmes toegepast op een CHT testprobleem voor zowel de hoge orde tijdsintegratie en algemeen gebruikelijke tweede orde methodes. Voor nauwkeurige, tijdsafhankelijke resultaten zijn de hoge orde schema’s efficiënter dan de tweede orde schema’s. De winst in rekentijd is groter als kleinere toleranties gewenst zijn.

Een ander onderwerp van dit proefschrift is de toepassing van de hoge orde ESDIRK schema’s op een cel-center, gecolloceerde, eindige volume discretisatie van de instationaire incompressibele Navier-Stokes vergelijkingen. In het bijzonder is een procedure voor de interpolatie van de snelheid van de cel naar de celwand (Rhie-Chow) geïntroduceerd, die de orde van de meertraps ESDIRK schema’s behoud. Daarbij wordt de invloed van iteratieve fouten op de orde van de tijdsintegratie geminimaliseerd door een iteratief algoritme te gebruiken. De resultaten van numerieke voorbeelden tonen het behoud van de tijdsintegratie orde aan.
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Chapter 1

Introduction

Thermal interaction of flows and structures, also referred to as conjugate heat transfer, arises in many engineering applications, where heat conduction in a solid is coupled to heat convection in an adjacent fluid [6, 13].

Heat removal strategies in the design of integrated circuits (IC) is an example of where CHT plays a crucial role. The expected life and reliability of a solid-state device depends very strongly on its operating temperature [31, 32]. Poor thermal design and management often leads to overheating, reduced performance, and failure; such issues become more pronounced as the feature sizes decrease and package densities increase. [31, 32] Many of the techniques which address thermal management in ICs are based on the thermal interaction of a working fluid with the IC package (such as micro-fluidic cooling).

Other examples of applications in which conjugate heat transfer is encountered include the thermal interaction between the fluid in a U-tube pipe with the surrounding soil in a geothermal heat exchanger system, the thermal interaction among various phases and materials in the mold region of a casting process, the cooling of gas turbine blades, interstitial thermal therapy, immersion lithography, spray technology, and design of HVAC (heating, ventilation, and air conditioning) systems.

Therefore, studying the thermal interaction of flows and structures is essential in enhancing the efficiency and/or safety of designs, and numerical simulations serve as a viable tool in this process. Conjugate heat transfer encountered in many engineering applications is unsteady and accurate determination of the transients is of great interest, given the additional physical insight provided into the evolution and dynamic response of the system [29]. Since time-accurate computations of conjugate heat transfer problems can be computationally expensive, the aim of this thesis is to develop flexible and efficient numerical procedures to reduce the computational work.
1.1 Overview

Due to the broad range of applications, there are many papers on the numerical modeling of CHT problems. They mainly differ by the degree to which the domains are coupled [14]. The monolithic and partitioned approaches are the two common methods for solving the thermal coupling of flows and structures.

In the monolithic method, the solution in the global domain is obtained by solving the governing equations within the subdomains as well as the interface equations simultaneously [6,13]; it requires the production of a single code specifically tailored for conjugate heat transfer problems [9,11]. In one approach, the equations of the fluid domain (continuity, momentum, and energy) are solved for the entire computational domain. By specifying the appropriate thermophysical properties in each region, the governing equations are reduced to the appropriate forms for each sub-domain; for example the velocity is forced to zero in the solid region by assigning very large viscosities [6,13]. When the finite volume approach is used for spatial discretization of the domains, the continuity of heat flux and temperature at interface of the subdomains are implicitly imposed through the harmonic mean formulation of the interface conductivities [27].

In the partitioned method on the other hand, a separate physics solver is associated with each subdomain [14]. The solution in the subdomains are coupled at the interface through a set of transmission conditions, and a coupling algorithm is required for the transfer of data between the subdomains. By solving the coupled problem in a partitioned manner, one can take advantage of the already existing efficient and highly optimized separate fluid and solid codes. Furthermore, it provides a flexible means of incorporating additional coupled phenomena among the subdomains (such as the mechanical coupling of fluids and structures).

There are also methods which can be placed between the fully partitioned and monolithic approaches [14]. For example, in [38], a single energy equation is used to solve for the temperature field in the entire computational domain. However, separate flow and structure solvers are associated with the different fluid and solid subdomains.

Time integration

In engineering applications, typically an implicit time integration is preferred over an explicit one in order to circumvent time step restrictions due to probable stiffness in the problem. Stiffness in a system can for example arise due to the nature of the governing equations or due to the generated grid (such as clustering of nodes near an area of interest [21]).

Performing time-accurate computations of transient CHT problems can be computationally demanding, in particular when low order time integration schemes are used. The obtained solution can suffer from low levels of temporal accuracy, and in order to increase the accuracy of the solution, smaller time steps must be taken. This results in an increase in the computational cost of solving the coupled problem.
As a potential solution, we consider the use of high order implicit time integration schemes for advancing the coupled problem in time. Computational efficiency of the high order time integration schemes relative to commonly used second order schemes has been demonstrated in \cite{1,41} for fluid flow computations, and in \cite{40} for the partitioned simulation of the mechanical coupling of flows and structures.

**Loosely and strongly coupled partitioned approaches**

In the partitioned approach, the interface equations are treated in a segregated manner where one of the interface equations is applied as a boundary condition for one subdomain, and the other as boundary condition for the second subdomain \cite{14}. In addition, by applying implicit time integration schemes to the subdomains, some or all of the interface terms are treated explicitly, depending on the arrangement with which the two coupled domains are solved (parallel (Block Jacobi) or sequential (Block Gauss-Seidel)). If at each time step (or stage of an implicit Runge-Kutta scheme), a single interface iteration (or fixed-point iteration) \cite{9,14} is performed, the partitioned algorithm is referred to as loosely-coupled, otherwise it is referred to as strongly-coupled. Depending on the strength of the thermal interaction between the subdomains, it is in general computationally more efficient to select either a loosely-coupled or strongly-coupled algorithm. In this thesis, the ratio of the thermal effusivities of the coupled domains, denoted by $\sigma$, is used as a measure of the strength of the thermal interaction: when $\sigma \ll 1$, the strength of the interaction is weak, and as $\sigma \to 1$ the strength of the interaction increases. (This is further discussed in Chapter 2).

Loosely-coupled solution algorithms can provide an efficient way of solving time-accurate weakly coupled CHT problems relative to the monolithic approach. In the literature, loosely-coupled solution algorithms with up to second order implicit time integration schemes are available (see \cite{2,7,11}). In this thesis, a loosely-coupled solution algorithm is presented in which a family of high order implicit-explicit (IMEX) Runge-Kutta schemes are used for time integration. The IMEX schemes consist of the explicit first-stage singly diagonally implicit Runge-Kutta (ESDIRK) schemes which are used for advancing the solution in time within each separate fluid and solid subdomain and equal order and number of stages explicit Runge-Kutta (ERK) schemes for explicit integration of part of the coupling terms. The IMEX schemes considered here were originally developed for solving time-accurate convection-diffusion-reaction (CDR) problems \cite{23} and later employed for the loosely coupled solution of the mechanical coupling of flows and structures \cite{40}.

In the partitioned approach using an implicit time integration scheme, as a result of the segregated treatment of the interface equations, the partitioned solution contains an additional source of error compared to the monolithic solution. This error is denoted as the partitioning error, $e(x,t)$. Due to the presence of the partitioning error, loosely-coupled algorithms are in particular susceptible to temporal order reduction and instability (not inherent to the monolithic approach) \cite{11}. For example, in the partitioned solution of a CHT problem, Birken et al. \cite{2} used the
second order SDIRK scheme to advance the coupled problem in time. In that paper, it was observed that the temporal order of accuracy of the partitioned solution obtained using a loosely-coupled solution algorithm, reduces to first order (the stage order). In order to retrieve the order of the time integration scheme, at each stage an additional implicit solve (a subiteration) was performed, hence increasing computational cost. By applying the stability theory of Godunov and Ryabenkii, Giles [11] analyzed the stability of a loosely-coupled solution algorithm where backward Euler (BDF1) was used for time integration. It was shown that the loosely-coupled algorithm should retain its stability for large Fourier numbers of the coupled domains, 
\[ d = \frac{\alpha \Delta t}{\Delta x^2} >> 1 \quad (\alpha : \text{thermal diffusivity}), \]
by the correct assignment of the interface boundary conditions (typically Dirichlet boundary condition should be imposed on the fluid side while Neumann boundary conditions on the solid side).

Therefore, in designing loosely-coupled solution algorithms, a number of issues needs to be considered. One, whether the design order of the time integration scheme is preserved without subiterating. Second, what are the stability properties of the algorithm; for practical computations, it is preferred that \( \Delta t \) is restricted by accuracy rather than stability. Given the multiple stages, applying analytical methods to study the accuracy and stability of the loosely-coupled IMEX schemes is not straightforward. However, because of similarities between the second stage of the loosely-coupled IMEX schemes and the predictor-corrector Crank-Nicolson scheme, analytical accuracy and stability analysis will be performed for the latter scheme. The accuracy and stability of the IMEX schemes will be investigated numerically, using the analytical results of the Crank-Nicolson scheme as reference.

As the thermal interaction between the domains becomes stronger, the stability and the temporal accuracy of the loosely-coupled schemes generally reduce. For such cases, it is more appropriate to use a strongly-coupled solution algorithm. Examples on the application of second order implicit time integration schemes to strongly-coupled solution algorithms can be found in [2, 14, 19]. In this thesis, a strongly-coupled solution algorithm is presented where the high order ESDIRK schemes are used for time integration. Interface iterations (subiterations) are performed (at each stage) to retain the stability and/or to increase the accuracy of the partitioned solution. The stability and rate of convergence of performing (Gauss-Seidel) subiterations at each stage of the ESDIRK schemes are analyzed analytically.

**Transient Navier-Stokes computations on collocated grids**
For the (loosely and/or strongly coupled) partitioned algorithms to preserve the temporal design order, it is necessary for the separate physics solvers to have the correct order behavior for the uncoupled simulations. For each physics solver, order reduction may occur as a result of the discretization method and/or the solution algorithm, among other factors. In this thesis, attention is given to the application of the high order ESDIRK schemes to the cell-centered collocated finite volume discretization of the unsteady incompressible Navier-Stokes (INS) equations, and to the segregated solve of the resultant fully discretized equations.
1.2. Aim

In many CFD packages, the cell-centered finite volume approach with collocated arrangement of the primitive variables is considered for discretization of the spatial operators in the INS equations. It is well known that a standard collocated grid finite volume method has convergence problems and spurious oscillations in the pressure field can occur which deteriorates the solution \cite{18, 28}. One widely used method in the literature and CFD packages to suppress the spurious modes is the interpolation procedure proposed by Rhie and Chow \cite{35}. This interpolation technique couples the pressure and velocity fields by formulating discretized momentum equations for the convective (cell-face) velocities \cite{8, 28}. The original interpolation method was proposed for steady-state computations and the temporal term was neglected in the derivation. In computing the solution to the unsteady INS equations (in particular using a class of segregated solution algorithms such as SIMPLE-like and PISO-like approaches), care should be taken in selecting the interpolation method, otherwise it will result in a time-step dependent steady-state solution, temporal order reduction, and/or temporal inconstancy (the solution deteriorates as time-step size is reduced). Reviews of the literature on this topic can be found in \cite{8} and \cite{33}. In this thesis, for the multi-stage ESDIRK schemes, a temporally order-preserving interpolation procedure is introduced. In addition, the details of an iterative pressure-based time advancing algorithm comprising the designed interpolation method are discussed.

1.2 Aim

The main objective of this thesis is to develop a flexible numerical approach to model transient fluid-solid thermal interactions (CHT) in a stable and efficient manner. The numerical approach should allow the use of much of the already existing efficient and highly optimized separate fluid and solid physics solvers. Furthermore, it should provide the possibility of incorporating additional coupled phenomena amongst the subdomains as well as within each subdomain. The partitioned approach provides this flexibility.

The high order implicit time integration schemes provide the possibility to increase the computational efficiency of solving transient CHT problems for a reasonable portion of the work-precision spectrum. However, when employed within the partitioned framework several key issues need to be considered.

- The partitioned approach should preserve the temporal design order of the applied high order time integration scheme. For loosely-coupled solution algorithms in particular, this should hold without the need for subiterations.

- In order to perform practical computations using the loosely-coupled approach, the time-step should be restricted by accuracy rather than stability. For the strongly-coupled approach, the stability and rate of convergence of performing subiterations needs to be analyzed.
• The high order time-integration schemes should be at least as efficient as the commonly used second order time integration schemes for reasonable temporal errors.

The secondary goal of this thesis is the development of a numerical algorithm for solving the incompressible Navier-Stokes on collocated grids using the ESDIRK schemes such that the design order of the time integration scheme is preserved.

In what follows, the equations governing conjugate heat transfer are discussed in chapter 2. In chapter 3, a brief overview of the ESDIRK and IMEX time integration schemes are presented. By noting similarities between the second stage of the IMEX schemes and the Crank-Nicolson scheme in chapter 3, the temporal accuracy and stability of the loosely-coupled solution algorithm in which the Crank-Nicolson scheme is used for time integration are analyzed in chapter 4. In chapter 5, the details of the loosely coupled solution algorithm in which the IMEX schemes are used for time integration are presented. Temporal order preservation and stability of the coupling algorithm is investigated numerically. Furthermore, the computational efficiency of the IMEX schemes relative to commonly used second order Crank-Nicolson and BDF2 schemes, in obtaining time-accurate solutions of a CHT-test case is considered. In chapter 6, the stability and rate of convergence of performing subiterations at each stage of the ESDIRK schemes are analyzed analytically. Numerical examples are then considered in order to validate the performed analytical stability analysis, and to investigate the computational efficiency of the algorithm relative to Crank-Nicolson and the high order loosely-coupled IMEX schemes. In chapter 7, the high order ESDIRK schemes are applied to collocated finite volume discretization of unsteady INS equations. An iterative time advancing algorithm for solving the unsteady INS is presented where by using an appropriate temporally consistent face-velocity interpolation, the temporal design order is preserved. In chapter 8, conclusions are drawn with respect to the developed numerical procedures. Furthermore, recommendations are made with respect to future directions for this work.
Chapter 2

Governing equations and model problem

In this chapter, the governing equations for modeling conjugate heat transfer are described. The presented model will be used to demonstrate the applicability of the partitioned algorithms, to validate the performed analytical stability analysis, and to investigate the computational efficiency of the high order time integration schemes. Furthermore, a one–dimensional model problem is introduced which will be used to discuss the details of the loosely-coupled solution algorithm and to analyze its accuracy and stability. In addition, by considering the analytical solution to the 1–D model problem, the concepts of weak and strong thermal interactions are discussed, and a single parameter is suggested to be used as a measure of the strength of the thermal interaction.

2.1 CHT governing equations

In the conjugate heat transfer problem considered here, the fluid domain is modeled using the Boussinesq approximation of the Navier-Stokes system which in primitive variables is given by:

\[ \nabla \cdot \mathbf{u} = 0, \]  
\[ \frac{\partial \mathbf{u}}{\partial t} = -(\mathbf{u} \cdot \nabla)\mathbf{u} + \nu \nabla^2 \mathbf{u} - \nabla p - \beta g \mathbf{j} (T_f - T_{ref}), \]  
\[ \frac{\partial T_f}{\partial t} = -(\mathbf{u} \cdot \nabla)T_f + \frac{1}{(\rho c_p)_f} \nabla \cdot (k_f \nabla T_f), \]  

where \( \mathbf{u} \) is the velocity vector, \( p \) is the kinematic pressure, \( \nu \) the kinematic viscosity, \( T_f \) the temperature, \( k_f \) the thermal conductivity, \( c_{p,f} \) the heat capacity, \( \rho_f \) the density, \( \beta \) the thermal expansion coefficient of the fluid, \( g \) the acceleration due to gravity, and \( \mathbf{j} \) is a vector indicating the direction at which the gravity acts.
Chapter 2.

The solid domain is modeled using unsteady heat conduction:

\[
\frac{\partial T_s}{\partial t} = \frac{1}{(\rho c_p)_s} \nabla \cdot (k_s \nabla T_s). \tag{2.4}
\]

The governing equations are accompanied by appropriate initial and boundary conditions. For a well-posed problem, the continuity of the temperature and heat flux are imposed at the common interface of the domains:

\[
T_f(I, t) = T_s(I, t), \tag{2.5}
\]

\[
q_s(I, t) = q_f(I, t), \tag{2.6}
\]

where \(q_m(I, t) = -k_m \nabla T_m \cdot n\) with \(m\) the index of the subdomain, and \(n\) the outward normal to the interface.

To identify the governing parameters in the conjugate heat transfer problem described by (2.1)-(2.6), the equations are casted into the following dimensionless form (assuming constant material properties and that \(T_{ref} = T_C\)):

\[
\nabla \cdot U = 0, \tag{2.7}
\]

\[
\frac{\partial U}{\partial \tau} = -(U \cdot \nabla)U + Pr \nabla^2 U - \nabla P - j Pr Ra \theta_f, \tag{2.8}
\]

\[
\frac{\partial \theta_f}{\partial \tau} = -(U \cdot \nabla) \theta_f + \nabla^2 \theta_f, \tag{2.9}
\]

\[
\frac{\partial \theta_s}{\partial \tau} = \frac{\alpha_s}{\alpha_f} \nabla^2 \theta_s, \tag{2.10}
\]

\[
\theta_f(I, t) = \theta_s(I, t), \tag{2.11}
\]

\[
\nabla \theta_f \cdot n = \frac{k_s}{k_f} \nabla \theta_s \cdot n, \tag{2.12}
\]

where the following non-dimensionalization based on [43] is used (note \(p\) is kinematic pressure):

\[
\nabla = L_{ref} \nabla, \quad \tau = \frac{t \alpha_f}{L_{ref}^2}, \quad U = \frac{u L_{ref}}{\alpha_f}, \quad P = \frac{p L_{ref}^2}{\alpha_f^2}, \tag{2.13}
\]

\[
\theta_f = \frac{T_f - T_C}{T_H - T_C}, \quad \theta_s = \frac{T_s - T_C}{T_H - T_C}, \quad Ra = \frac{g \beta (T_H - T_C) L_{ref}^3}{\nu \alpha_f}, \quad Pr = \frac{\nu}{\alpha_f}.
\]

Based on the dimensionless form of the equations, it is observed that the ratio of the thermal conductivities of the domains (\(k_s/k_f\)), the ratio of thermal diffusivities of the domains (\(\alpha_s/\alpha_f\) where \(\alpha = k/\rho c_p\)), the Prandtl number (\(Pr = \nu/\alpha_f\)), and the Rayleigh number (\(Ra = g^3(T_H - T_C)L_{ref}^3/\nu \alpha_f\)) are the governing parameters of the problem.
2.2 Model Problem

In this section, the description of a one-dimensional model problem is presented which will be used to discuss the details of the loosely-coupled solution algorithm and to analyze its accuracy and stability. The model problem has been commonly used in the literature (for example [11, 14, 36]) to analyze stability of numerical algorithms for thermal coupling of domains. The model problem consists of thermal coupling of two domains $\Omega_1 = [-L_1, 0]$ and $\Omega_2 = [0, L_2]$, with their common interface $I$ at $x = 0$. The governing equation within each sub-domain is transient linear heat conduction. For simplicity, each sub-domain has constant material properties. The initial boundary value problem is given by:

\[
(p c_p) \frac{\partial T_m(x, t)}{\partial t} = -k_m \frac{\partial q_m(x, t)}{\partial x}, \quad m = 1, 2, \tag{2.14}
\]

\[
q_m(x, t) = -k_m \frac{\partial T_m(x, t)}{\partial x}, \quad m = 1, 2, \tag{2.15}
\]

\[
T_1(x = -L_1, t) = T_{1,lbc}, \tag{2.16}
\]

\[
T_2(x = L_2, t) = T_{2,rbc}, \tag{2.17}
\]

\[
T_2(I, t) = T_1(I, t), \tag{2.18}
\]

\[
q_1(I, t) = q_2(I, t), \tag{2.19}
\]

\[
T_1(x, t = 0) = T_{1,lbc}, \tag{2.20}
\]

\[
T_2(x, t = 0) = T_{2,rbc}, \tag{2.21}
\]

where $T_m$ and $q_m$ respectively represent the temperature and heat flux fields within each domain, with $m$ the index of the subdomain. The non-interface boundaries are constant Dirichlet conditions.

An analytical solution to the model problem can be obtained in terms of Fourier series using the method of separation of variables (see [30, chap.6]). However, a simpler form of the analytical solution can be obtained if the two coupled domains are considered as semi-infinite. The non-interface boundary conditions ($x \rightarrow \pm \infty$) are given by:

\[
T_1(x \rightarrow -\infty, t) = T_{1,lbc}, \tag{2.22}
\]

\[
T_2(x \rightarrow \infty, t) = T_{2,rbc}. \tag{2.23}
\]

The solution to this coupled problem is given by ([4, 10]):

\[
T_1 = T_{1,lbc} + \frac{e_2}{e_1} \left( T_{2,rbc} - T_{1,lbc} \right) erfc \left( \frac{|x|}{\sqrt{4\alpha_1 t}} \right), \tag{2.24}
\]

\[
T_2 = T_{2,rbc} - \frac{1}{1 + \frac{e_2}{e_1}} \left( T_{2,rbc} - T_{1,lbc} \right) erfc \left( \frac{x}{\sqrt{4\alpha_2 t}} \right), \tag{2.25}
\]
where \( e_m = \sqrt{k_m \rho_m c_{p,m}} \) is the thermal effusivity within each subdomain. The interface temperature remains constant with time and is given by:

\[
T_{I,exact} = \frac{T_{1,lbc} + \frac{e_2}{e_1} T_{2,rbc}}{1 + \frac{e_2}{e_1}}, \quad (2.26)
\]

while the heat flux at the interface decreases with time and is given by:

\[
q_{I,exact} = \frac{T_{2,rbc} - T_{1,lbc}}{1 + \frac{e_2}{e_1}} \frac{e_2}{\sqrt{\pi t}}. \quad (2.27)
\]

It is noted that the ratio of the thermal effusivities of the coupled domains,

\[
\sigma = \frac{e_2}{e_1} = \frac{\sqrt{k_2 \rho_2 c_{p,2}}}{\sqrt{k_1 \rho_1 c_{p,1}}} = \frac{k_2}{k_1} \frac{\sqrt{\alpha_1}}{\sqrt{\alpha_2}}, \quad (2.28)
\]

is one of the governing parameters of the coupled problem. Assuming that \( \sigma \ll 1 \), the variation of the temperature field in \( \Omega_1 \) from the imposed initial condition is small, and changes mainly occur in \( \Omega_2 \). As this ratio approaches unity, both the subdomains experience temperature variations. Therefore, it appears that \( \sigma \) can be used as a measure of the strength of the thermal interaction: when \( \sigma \ll 1 \), the strength of the interaction is weak, and as \( \sigma \rightarrow 1 \) the strength of the interaction increases.
Chapter 3

Space discretization and Time integration

In this chapter, a brief overview of the high order time integration schemes which will be used for advancing the solution to the coupled problem in time is presented. We discuss a family of implicit-explicit (IMEX) Runge-Kutta schemes which will be used in the loosely-coupled solution algorithm, and a family of implicit Runge-Kutta (IRK) schemes which will be used in the strongly-coupled solution algorithm.

The method of lines [25] is used to solve the PDEs, in which the spatial operators are discretized first in order to obtain the semi-discrete form of the equations. In the thesis, unless otherwise mentioned, the cell-centered finite volume approach is used for spatial discretization of the subdomains. The one dimensional model problem described in section 2.2 will be used to briefly demonstrate the approach. Noting that the global domain Ω is split into Ω₁ and Ω₂, prior to space discretization, interface boundary conditions must be imposed on the two subdomains.

3.1 Imposing interface boundary conditions

In this thesis, the Dirichlet-Neumann transmission conditions are considered for coupling the two domains at the interface. For partitioned algorithms, the stability of the coupling algorithm depends on the correct assignment of the interface conditions. Using a two-dimensional variant of the model problem in section 2.2, Henshaw and Chand [14] analyzed the stability and the rate of convergence of Dirichlet-Neumann interface iterations, using the θ scheme for time integration and without any particular assumption on the spatial discretization. They arrived at the following estimate for the rate of convergence of the iterations for the smooth components of the solution:

\[ \Phi \approx \frac{k_2}{k_1} \sqrt{\frac{\alpha_1}{\alpha_2}}, \]  

(3.1)
where \( k_m \) and \( \alpha_m \) (with \( m = 1, 2 \)) represent the thermal conductivity and thermal diffusivity of each subdomain. The estimate was obtained by imposing the Dirichlet (temperature) condition on \( \Omega_2 \) with the interface temperature of \( \Omega_1 \) being prescribed as its value, and the Neumann (the heat flux) condition on \( \Omega_1 \) with the interface heat flux of \( \Omega_2 \) being prescribed as its value. Performing interface iterations based on the assigned interface boundary conditions is stable if,

\[
\Phi < 1,
\]

otherwise the two interface boundary conditions must be interchanged.

While the criterion (3.2) has been obtained for a strongly-coupled solution algorithm, it can also be used as a criterion for imposing interface boundary conditions for loosely-coupled solution algorithms; that is, for stability of a loosely-coupled partitioned algorithm, satisfying (3.2) is necessary but might not be sufficient. It is interesting to note that the expression in (3.1) is equal to the ratio of thermal effusivities of the coupled domains, i.e. \( \Phi = \sigma \). Therefore, for stability, the domain with the higher \( \sigma \) is assigned the Neumann condition and the one with the lower \( \sigma \) the Dirichlet condition.

Here, it is assumed that based on the material properties of the two subdomains, the imposed interface boundary conditions satisfy the criterion (3.2), i.e. the temperature condition is assigned to \( \Omega_2 \) and the heat flux condition to \( \Omega_1 \).

### 3.2 Space discretization and Semi-Discrete Form

With the interface boundary conditions imposed, the two domains are discretised in space using the cell-centered finite volume (CFV) method (see Fig. 3.1).

![Figure 3.1: Discretization of \( \Omega_1 \) and \( \Omega_2 \) subdomains using CVF.](image)

Applying the volume integral form of the governing equation (2.14) to each control volume results in:

\[
(\Delta x \rho c_p)m \frac{d}{dt}T_{m,j} = -q_m|_{j-1/2}^{j+1/2} \quad m = 1, 2,
\]

where for simplicity cells of equal size are used within each subdomain. Substituting (2.15) into (3.3) for \( q_m \), and using central difference to approximate the temperature gradients at the cell faces, the semi-discrete form of equation (2.14) for the interior
3.2. Space discretization and Semi-Discrete Form

cells, after some rearrangement, is given by:

\[
(\Delta x \rho c_p)_m \frac{d}{dt} T_{m,j} = \frac{k_m}{\Delta x_m} T_{m,j+1} - \frac{2k_m}{\Delta x_m} T_{m,j} + \frac{k_m}{\Delta x_m} T_{m,j-1} = F_{m,j} \quad m = 1, 2,
\]

where \( F_{m,j} \) is the cell-residual obtained as a result of discretizing the governing equation in space.

In \( \Omega_2 \), the discretization of the cell adjacent to the interface, \( T_{2,1} \), is given by (noting that one-sided differencing is used to approximate the temperature gradient in the interface heat flux \( q_{2,I} = -(k_2 \frac{\partial T_2}{\partial x})|_I \)):

\[
(\Delta x \rho c_p)_2 \frac{d}{dt} T_{2,1} = \frac{k_2}{\Delta x_2} (T_{2,2} - T_{2,1}) - \frac{k_{2,I}}{\Delta x_{2,b}} (T_{2,1} - T_{2,I}) = F_{2,1},
\]

where \( T_{2,I} \) is the interface temperature on the side of \( \Omega_2 \) and \( \Delta x_{2,b} = \frac{\Delta x_{2,1}}{2} \) is the distance from the cell center of \( T_{2,1} \) to the interface. \( k_{2,I} \) is the interface conductivity on the side of \( \Omega_2 \) and unless otherwise mentioned is equal to constant value of \( k_2 \) prescribed to the complete field (\( \Omega_2 \)). Rewriting (3.5), we obtain:

\[
(\Delta x \rho c_p)_2 \frac{d}{dt} T_{2,1} = \frac{k_2}{\Delta x_2} (T_{2,2} - T_{2,1}) - \left( \frac{k_2}{\Delta x_2} + \frac{k_{2,I}}{\Delta x_{2,b}} \right) T_{2,1} + f_{21} = F_{2,1},
\]

where \( f_{21} = \frac{k_{2,I}}{\Delta x_{2,b}} T_{2,I} \) is the contribution from the Dirichlet boundary (interface) condition. The value of the interface temperature is obtained by prescribing the temperature of the interface node in \( \Omega_1 \) as its value \( T_{2,I} = T_{1,I} \). However, it is noted that \( \Omega_1 \) does not have a node at the interface. Therefore, in order to solve the coupled system an approximation to the interface temperature is required. Here, linear extrapolation from cells in \( \Omega_1 \) close to the interface is used to approximate the interface temperature:

\[
T_{1,I} = \mu T_{1,-2} + \xi T_{1,-1},
\]

where \( \mu = -1/2 \) and \( \xi = 3/2 \) for a uniform grid in \( \Omega_1 \).

In \( \Omega_1 \), the discretization of the cell adjacent to the interface, \( T_{1,-1} \), is:

\[
(\Delta x \rho c_p)_1 \frac{d}{dt} T_{1,-1} = -q_{1,I} - \frac{k_1}{\Delta x_1} (T_{1,-1} - T_{1,-2}) = F_{1,-1},
\]

where \( q_{1,I} \) is the interface heat flux on the side of \( \Omega_1 \) and based on the Dirichlet-Neumann formulation, the interface heat flux of \( \Omega_2 \) is prescribed as its value:

\[
q_{1,I} = q_{2,I} = -\frac{k_{2,I}}{\Delta x_{2,b}} (T_{2,1} - T_{2,I}).
\]
The semi-discrete form of the coupled problem can be expressed by the following two coupled ODE systems:

\[ M_1 \frac{dT_1}{dt} = F_1(T_1, q_1, I, t) \quad , \tag{3.10} \]
\[ M_2 \frac{dT_2}{dt} = F_2(T_2, T_2, I, t) \quad , \tag{3.11} \]

where, the vectors \( T_1 \) and \( T_2 \) contain the discrete solution in the FV cells, \( M_1 \) and \( M_2 \) are diagonal matrices containing the product of the cells’ volumetric heat capacities \( (\rho c_p)_m \) with the cell volumes. \( F_1 \) and \( F_2 \) are the residual vectors defined by:

\[ F_1 = A_1 T_1 - q_1 b_1 + f_1 \quad , \tag{3.12} \]
\[ F_2 = A_2 T_2 + f_{21} b_2 + f_2 \quad , \tag{3.13} \]

where, \( A_m (m = 1, 2) \) represents the discretization of the diffusion term, and \( f_m \) is a vector containing the contribution of the non-interface boundary. The vector \( b_m \) contains zero entries except for the discretization of the cell next to the interface for which its entry is 1. As (3.10)-(3.11) demonstrate, the coupling between the two systems is through the interface temperature \( T_2 \) and heat flux \( q_1 \).

### 3.3 ESDIRK schemes

In this thesis, for each subdomain, the ESDIRK schemes are considered for time integration which can be made of arbitrary high order while retaining the L-stability property. While BDF1 and BDF2 are L-stable, the Crank-Nicolson scheme is only A-stable. It is possible to construct higher order BDF methods, but they are only \( L(\alpha) \) stable and their stability region drops as the order of the scheme is increased (see [12]). For an ODE system of the form \( M \frac{dT}{dt} = F(T, t) \), the solution at each stage of the ESDIRK scheme can be written as:

\[ MT^{(k)} = MT^n + \Delta t \sum_{i=1}^{k} a_{ki}^{I} F(T^{(i)}, t^n + c_i \Delta t) = MT^n + \Delta t \sum_{i=1}^{k} a_{ki}^{I} F^{(i)}, \tag{3.14} \]

where \( a_{ki}^{I} \) are the stage weights, and \( c_i = \sum_j a_{ij}^{I} \) are the quadrature nodes of the scheme, \( t^{(i)} = t^n + c_i \Delta t \). The solution at the next time level is obtained by:

\[ T^{n+1} = T^n + M^{-1} \Delta t \sum_{i=1}^{s} b_i F^{(i)}, \tag{3.15} \]

where \( b_i \) are the scheme’s main weights with \( \sum_i b_i = 1 \), and \( s \) is the number of stages. In this thesis, stiffly accurate ESDIRK schemes are considered where \( a_{si}^{I} = b_i \).
and thus the solution of the last stage is equal to the solution of the next time-level, $T^{n+1} = T^{(s)}$. Therefore, when a fully coupled approach is used to solve the coupled problem (performing interface iterations until convergence to the monolithic solution), computing (3.15) becomes unnecessary. Since the ESDIRK schemes have reduced stage orders, they are susceptible to order-reduction in the presence of substantial stiffness (see [3]). The coefficients and weights are usually arranged in a Butcher tableau (see Table 3.1). In this thesis, the high order ESDIRK schemes developed in Kennedy and Carpenter [23] are used. For the ESDIRK schemes, as the name implies, the diagonal coefficients are equal ($a_{kk} = \gamma$). Furthermore, it is possible to incorporate the ESDIRK schemes into solvers which already include the Backward Euler, since from an implementation viewpoint, each stage of the ESDIRK scheme resembles the BDF1 scheme with a source term.

### 3.4 Additive Runge-Kutta schemes

In solving time-accurate advection-diffusion-reaction problems, where separable stiff and non-stiff components are identifiable, Kennedy and Carpenter [23] present a family of high order IMEX (additive) Runge-Kutta schemes where the ESDIRK schemes are used for integrating the stiff components of the problem (to retain stability) and ERK schemes (which are computationally less expensive than the corresponding implicit schemes) are used for integrating the non-stiff components of the problem. In order to be consistent with the ESDIRK schemes, the introduced ERK schemes have the same order and number of stages as the ESDIRK schemes (they have the same weight factors $b_i$ and $c_i$ coefficients). For the time-step solution to have the designed high order accuracy, evaluating (3.15) is necessary. In this thesis, the coefficients of the implicit ESDIRK schemes are denoted by $a^I_{ki}$ and that of the ERK schemes by $a^E_{ki}$ as shown in Table 3.1.

Analogously, in solving unsteady CHT problems using the loosely-coupled solution algorithm, the coupling terms between the fluid and solid subdomains are assumed as separable components which can be integrated with the explicit ERK schemes; the fluid and solid systems are integrated with the implicit ESDIRK schemes. This approach follows from [40] where the mechanical coupling of fluids and structures is considered. Furthermore, similar to [40], the high order IMEX schemes developed in [23] are used for time integration. This class of IMEX schemes has also been used in [21] to overcome geometry induced stiffness in a single (fluid) domain; the non-stiff portion of the domain is integrated using ERK schemes and the stiff portions using the ESDIRK schemes.

By expressing the predictor-corrector $\theta$ scheme, used in [22] for solving unsteady CHT problems, in terms of a two-stage IMEX scheme (its Butcher tableau is given in Table 3.2), similarities can be observed between the $\theta$ scheme with $\theta = 0.5$ (Crank-Nicolson) and the second stage of the high order IMEX schemes. For the second stage of the IMEX schemes, the coefficients of the corresponding ESDIRK and ERK
Table 3.1: A four stage additive RK method consisting of an ESDIRK and ERK scheme.

\[
\begin{array}{c|cccc}
  c_1 & 0 & 0 & 0 & 0 \\
  c_2 & a_I^{21} & a_I^{22} & 0 & 0 \\
  c_3 & a_I^{31} & a_I^{32} & a_I^{33} & 0 \\
  c_4 & a_I^{41} & a_I^{42} & a_I^{43} & a_I^{44} \\
\end{array}
\begin{array}{c|cccc}
  b_1 & b_2 & b_3 & b_4 \\
\end{array}
\begin{array}{c|cccc}
  c_1 & 0 & 0 & 0 & 0 \\
  c_2 & a_E^{21} & 0 & 0 & 0 \\
  c_3 & a_E^{31} & a_E^{32} & 0 & 0 \\
  c_4 & a_E^{41} & a_E^{42} & a_E^{43} & 0 \\
\end{array}
\begin{array}{c|cccc}
  b_1 & b_2 & b_3 & b_4 \\
\end{array}
\]

schemes are respectively given by \(a_I^{21} = \gamma\), \(a_I^{22} = \gamma\), and \(a_E^{21} = 2\gamma\) and those of the (predictor-corrector) Crank-Nicolson scheme are \(a_{21} = 0.5\), \(a_{22} = 0.5\), \(a_{21}^E = 1\).

\[
\begin{array}{c|ccc}
  0 & 0 & 0 \\
  1 & 1 - \theta & \theta \\
  1 - \theta & \theta \\
\end{array}
\begin{array}{c|ccc}
  0 & 0 & 0 \\
  1 & 1 & 0 \\
  1 - \theta & \theta \\
\end{array}
\]

Table 3.2: Butcher tableau for the predictor-corrector \(\theta\) scheme.

In the next chapters, partitioned algorithms for solving unsteady conjugate heat transfer will be introduced where the presented high order time integration schemes are applied. Furthermore, the stability, temporal accuracy, and computational efficiency of the algorithms will be analyzed.
Chapter 4

Accuracy and stability of predictor-corrector Crank-Nicolson


As mentioned earlier in the introduction, in designing loosely-coupled solution algorithms, the temporal order preservation of the algorithm *without the need for subiterations*, and its stability properties need to be analyzed. However, noting that the IMEX schemes consist of multiple stages, it is not straightforward to study analytically the accuracy and stability of the resultant loosely-coupled algorithm. However, based on the earlier observation in section 3.4 regarding the similarities between the second stage of the IMEX schemes and the $\theta$ scheme with $\theta = 0.5$, in this chapter we will proceed with performing accuracy and stability analyses for the loosely-coupled partitioned algorithm in which the Crank-Nicolson scheme is used for time integration. To validate the performed analytical accuracy and stability analyses, numerical examples are considered. The accuracy and stability of the IMEX schemes will be investigated numerically in the next chapter; the results will be compared to the conclusions of the analysis for the Crank-Nicolson scheme.

4.1 Space discretization

The one dimensional model problem described in section 2.2 is used to discuss the details of the loosely-coupled solution algorithm and to analyze its accuracy and stability. The global domain $\Omega$ is split into $\Omega_1$ and $\Omega_2$, and it is assumed that the
criterion (3.2) is satisfied by assigning the temperature condition to Ω₂ and the heat flux condition to Ω₁. The method of lines [25] is used to solve the PDEs. To carry out the analytical analysis, it is more convenient to consider the vertex-centered finite volume (VFV) method for spatial discretization of the subdomains (see Fig. 4.1). Therefore, a brief overview of this spatial discretization is presented below.

![Figure 4.1: Discretization of Ω₁ and Ω₂ subdomains using FVF.](image)

Applying the volume integral form of the governing equation (2.14) to each control volume results in:

\[(\Delta x \rho c_p)_m \frac{d}{dt} T_{m,j} = -q_{m,j+1/2} \quad m = 1, 2,\]  

(4.1)

where for simplicity cells of equal size are used within each subdomain (for the interface cell, \(\Delta x_1\) is replaced with \(\frac{\Delta x_1}{2}\)).

Substituting (2.15) for \(q_m\) into (4.1) and using central difference to approximate the temperature gradients at the cell faces, the semi-discrete form of equation (2.14) for the interior cells, with some rearrangements is given by:

\[(\Delta x \rho c_p)_m \frac{d}{dt} T_{m,j} = \frac{k_m}{\Delta x_m} T_{m,j+1} - \frac{2k_m}{\Delta x_m} T_{m,j} + \frac{k_m}{\Delta x_m} T_{m,j-1} = F_{m,j} \quad m = 1, 2,\]  

(4.2)

where \(F_{m,j}\) is the cell-residual obtained as a result of discretizing the governing equation in space.

In Ω₂, the value of the interface temperature \(T_{2,I} = 1\) is obtained by prescribing the temperature of the interface node in Ω₁ as its value, i.e. \(T_{2,0} = T_{1,0}\).

In Ω₁, the discretization of \(T_{1,0}\) is given by:

\[\frac{\Delta x}{2} \rho c_p \frac{d}{dt} T_{1,0} = -q_{1,0} - \frac{k_1}{\Delta x_1} (T_{1,0} - T_{1,-1}) = F_{1,0},\]  

(4.3)

where \(q_{1,I} = 0\) is obtained by prescribing \(q_{2,0}\) as its value:

\[q_{1,0} = q_{2,0} = -\frac{k_2}{\Delta x_2} (T_{2,1} - T_{2,0}).\]  

(4.4)

The semi-discrete form of the coupled problem can be expressed by the following
two coupled ODE systems:

\[ M_1 \frac{d}{dt} T_1 = \mathcal{F}_1(T_1, q_{1,\mathcal{I}}, t) , \]  
\[ M_2 \frac{d}{dt} T_2 = \mathcal{F}_2(T_2, T_{2,\mathcal{I}}, t) , \]

where as discussed earlier, the interface equations have been applied as boundary conditions to the subdomains:

\[ T_{2,\mathcal{I}} = T_{1,0} , \]  
\[ q_{1,\mathcal{I}} = -\frac{k_2}{\Delta x_2} (T_{2,1} - T_{2,0}) . \]

The vectors \( T_1 \) and \( T_2 \) contain the discrete solution in the FV cells, \( M_1 \) and \( M_2 \) are diagonal matrices containing the product of the cells’ volumetric heat capacities \( ((\rho c_p)_m) \) with the cell volumes. The residual vectors \( \mathcal{F}_1 \) and \( \mathcal{F}_2 \) are defined by:

\[ \mathcal{F}_1 = A_1 T_1 - q_{1,\mathcal{I}} b_1 + f_1 , \]  
\[ \mathcal{F}_2 = A_2 T_2 + T_{2,\mathcal{I}} b_2 + f_2 , \]

where, \( A_m \) (\( m = 1, 2 \)) represents the discretization of the diffusion term, and \( f_m \) is a vector containing the contribution of the non-interface boundary. Vector \( b_1 \) contains zero entries except for the discretization of the cell at the interface for which its entry is 1. Similarly, vector \( b_2 \) contains zero entries except for the discretization of the cell next to the interface, \( T_{2,1} \), for which its entry is \( \frac{k_2}{\Delta x_2} \). As (4.5)-(4.6) demonstrate, the coupling between the two systems is through the interface temperature \( T_{2,\mathcal{I}} \) and heat flux \( q_{1,\mathcal{I}} \).

### 4.2 Solution algorithm

In the following sections, the details and properties (accuracy and stability) of the loosely coupled solution algorithm are discussed using the theta scheme (with \( 0.5 \leq \theta \leq 1 \)) for time integration. The Crank-Nicolson scheme is then considered by using \( \theta = 0.5 \).

Application of the \( \theta \) scheme to (4.5)-(4.6) yields,

\[ \frac{M_1}{\Delta t} (T_1^{n+1} - T_1^n) = \theta (A_1 T_1^{n+1} - q_{1,\mathcal{I}}^{n+1} b_1 + f_1^{n+1}) + (1 - \theta) \mathcal{F}_1^n , \]  
\[ \frac{M_2}{\Delta t} (T_2^{n+1} - T_2^n) = \theta (A_2 T_2^{n+1} + T_{2,\mathcal{I}}^{n+1} b_2 + f_2^{n+1}) + (1 - \theta) \mathcal{F}_2^n , \]

where both the interface conditions (4.7) and (4.8) are treated implicitly,

\[ T_{2,\mathcal{I}}^{n+1} = T_{1,0}^{n+1} , \]  
\[ q_{1,\mathcal{I}}^{n+1} = -\frac{k_2}{\Delta x_2} (T_{2,1}^{n+1} - T_{2,0}^{n+1}) . \]
The monolithic solution to the coupled problem at time level \( t^{n+1} \) is denoted by \( T^{n+1}_m \). We will approximately solve the coupled implicit equations (4.11)-(4.12) for \( T^{n+1}_m \), by considering a sequential solve of the coupled subdomains – Block Gauss-Seidel (BGS). Furthermore, to improve the temporal accuracy of the solution, a predictor-corrector approach is followed.

In the predictor step, an initial approximation to \( T^{n+1}_m \) is computed by performing a single BGS iteration (here we consider integrating \( \Omega_1 \) first and is denoted by BGS-12); this intermediate temperature field is denoted by \( T^*_m \). In computing \( T^*_m \), the interface heat flux at \( t^n \) is used as a prediction for \( q^{n+1}_{1,\bar{x}} \):

\[
\frac{M_1}{\Delta t} (T^*_1 - T^n_1) = \theta (A_1 T^*_1 - q^{n}_{1,\bar{x}} b_1 + f^{n+1}_1) + (1 - \theta) F^*_1. \quad (4.15)
\]

With \( T^*_1 \) computed, we assign \( T^*_2 = T^*_1,0 \) and solve for \( T^*_2 \):

\[
\frac{M_2}{\Delta t} (T^*_2 - T^n_2) = \theta (A_2 T^*_2 + T^*_2,0 b_2 + f^{n+1}_2) + (1 - \theta) F^*_2. \quad (4.16)
\]

With the intermediate temperature field \( T^*_m \) computed, the interface condition is updated:

\[
q^*_1,\bar{x} = -\frac{k_2}{\Delta x_2}(T^*_2,1_T - T^*_2,0), \quad (4.17)
\]

where \( T^*_2,0 = T^*_1,0 \). The residual vectors \( F^*_1 \) and \( F^*_2 \) are computed next using (4.9) and (4.10) respectively. In the corrector step, an explicit update of the temperature field is computed:

\[
\frac{M_1}{\Delta t} (T^{**}_1 - T^n_1) = \theta F^*_1(T^*_1, q^*_1,\bar{x}, t^{n+1}) + (1 - \theta) F^*_1, \quad (4.18)
\]

\[
\frac{M_2}{\Delta t} (T^{**}_2 - T^n_2) = \theta F^*_2(T^*_2, T^*_2,\bar{x}, t^{n+1}) + (1 - \theta) F^*_2. \quad (4.19)
\]

The pseudocode of the algorithm is shown in Algorithm 1. The solution procedure is the same when the coupled problem is solved by integrating \( \Omega_2 \) first (BGS-21). However, after obtaining the solution field in the predictor step, both the interface conditions are updated \( (T^*_2,0 = T^*_1,0, \text{ and } (4.17)) \).

**Algorithm 1** loosely-coupled predictor-corrector algorithm; using BGS-12

1. Assign \( q^n_{1,\bar{x}} \) to \( \Omega_1 \) and solve for \( T^*_1 \), (4.15).
2. Assign \( T^*_2,\bar{x} \) to \( \Omega_2 \) and solve for \( T^*_2 \), (4.16).
3. Update interface equation (4.17).
4. Compute residual vector \( F^*_m \), (4.9)–(4.10).
5. Explicitly update the temperature fields using (4.18)–(4.19).
4.3 Temporal accuracy analysis

The partitioned solution contains two temporal error components: the time integration error and the partitioning error. The time integration error is related to discretization of the time derivative, and the partitioning error appears as a result of segregated treatment of the interface equations. For the solution algorithm to preserve the design order of the time integration scheme, the partitioning error needs to be at least of the same order as time integration error. In this section the temporal accuracy of the loosely-coupled solution algorithm in solving the model problem is assessed.

The accuracy analysis follows that of Issa [15] in which the temporal order of accuracy of the PISO algorithm for solving the incompressible Navier-Stokes equations is analyzed. The analysis is based on using the one-step error [25] defined as the error which is introduced in one time step assuming that the previous solutions are equal to the exact solutions. For example, for a second order time integration scheme, the temporal error introduced in one time step is of \( O(\Delta t^3) \).

To perform the accuracy analysis, let \( \epsilon_m \) (with \( m = 1, 2 \)) define the partitioning error in the solution field of the coupled domains,

\[
\epsilon_m^w = T_m^{n+1} - T_m^w, \quad m = 1, 2
\] (4.20)

where \( w \) stands for any one of the superscripts \( * \) and \( ** \). Similarly, \( \epsilon_q \) defines the partitioning error in satisfying the interface heat flux:

\[
\epsilon^q = q_{1, I}^{n+1} - q_{1, I},
\] (4.21)

and \( \epsilon_T \) defines the partitioning error in satisfying the interface temperature:

\[
\epsilon^T = T_{2, I}^{n+1} - T_{2, I},
\] (4.22)

where \( l \) in (4.21) stands for any one of the superscripts \( n \) and \( * \).

We begin the accuracy analysis by subtracting (4.15) and (4.16) from their corresponding monolithic discretizations (4.11) and (4.12) to obtain (4.23) and (4.24):

\[
\frac{M_1}{\Delta t}(\epsilon^*_1) = \theta(A_1 \epsilon^*_1 - \epsilon^q_{1, I} b_1),
\] (4.23)

\[
\frac{M_2}{\Delta t}(\epsilon^*_2) = \theta(A_2 \epsilon^*_2 + \epsilon^T_{2, I} b_2).
\] (4.24)

where \( \epsilon^q \) = \( q_{1, I}^{n+1} - q_{1, I}^{n} \) and \( \epsilon^T \) = \( T_{2, I}^{n+1} - T_{2, I}^{n} \). Using Taylor series expansion to approximate \( q_{1, I}^{n+1} \), the partitioning error \( \epsilon^q_{1, I} \) can be expressed by:

\[
\epsilon^q_{1, I} = q_{1, I}^{n+1} - q_{1, I}^{n} = q_{1, I}^{n} + O(\Delta t) - q_{1, I}^{n} = O(\Delta t).
\] (4.25)

Substituting the result into (4.23), it follows that:

\[
\epsilon^*_1 = O(\Delta t^2),
\] (4.26)
and accordingly (noting that $\mathbf{e}_{1,0}^* = \mathbf{e}_{1,0}^*$ which follows from $T_{2,0}^* = T_{1,0}^*$):

$$\mathbf{e}_{1}^* = O(\Delta t^3).$$

(4.27)

Therefore, at the end of the predictor step, the global temperature field ($\mathbf{T}_n^*$) obtained using the partitioned scheme is of $O(\Delta t^2)$ while it should be of $O(\Delta t^3)$ and order reduction occurs for the case $\theta = 0.5$ (Crank-Nicolson). Subtracting the updated interface heat flux in (4.17) from the corresponding monolithic one, we have:

$$\mathbf{e}_{1}^* \mathbf{q} = -\frac{k_2}{\Delta x_2} (\mathbf{e}_{2,1}^* - \mathbf{e}_{2,0}^*),$$

(4.28)

Subtracting (4.18)-(4.19) from its corresponding monolithic discretization (4.11)-(4.12), we have:

$$\begin{align*}
\frac{M_1}{\Delta t} (\mathbf{e}_{1}^{**}) &= \theta (A_1 \mathbf{e}_{1}^* + \mathbf{e}_{1}^* \mathbf{b}_1), \\
\frac{M_2}{\Delta t} (\mathbf{e}_{2}^{**}) &= \theta (A_2 \mathbf{e}_{2}^* + \mathbf{e}_{2}^* \mathbf{b}_2).
\end{align*}$$

(4.29) (4.30)

In (4.28), $\mathbf{e}_{2,1}^*$ is of $O(\Delta t^3)$ (based on (4.27)) and $\mathbf{e}_{2,0}^*$ where $\mathbf{e}_{2,0}^* = \mathbf{e}_{1,0}^*$ is of $O(\Delta t^2)$ (based on (4.26)). Therefore, the leading error term in (4.28) is of $O(\Delta t^2)$, and hence $\mathbf{e}_{2}^* = O(\Delta t^2)$. As a result, $\mathbf{e}_{1}^{**} = O(\Delta t^3)$ and $\mathbf{e}_{2}^{**} = O(\Delta t^3)$ similar to $\mathbf{e}_{2}^*$. Thus, after performing one corrector step, the temperature field $\mathbf{T}_m^{**}$ has the same order of accuracy as the time integration scheme. Each additional update of both the interface conditions followed by a corrector step, will increase the order of accuracy of the partitioning error (in the solution field and the interface quantities) by one (for example after a second corrector step one obtains: $\mathbf{e}_{2}^{**} = O(\Delta t^3),\ \mathbf{e}_{1}^{***} = O(\Delta t^4)$ and $\mathbf{e}_{2}^{***} = O(\Delta t^4)$). However, as pointed out in Issa [15], additional corrector steps will not influence the temporal order of accuracy of the partitioned solution, once the order of accuracy of the partitioning error becomes higher than that of the time integration error. Moreover, due to the explicit nature of the corrector steps, it can be expected that the stability of the coupling algorithm reduces as the number of the corrector steps increases.

In general, one is interested in the long term behavior of the partitioned solution, as in practice many time steps are taken. In the results section, numerical examples are considered where computations are carried out over many time-steps. The temporal convergence of the solution fields are investigated and compared with the conclusions of the one-step accuracy analysis.

### 4.4 Stability analysis

In this section, the stability of the loosely-coupled solution algorithm (presented in section 4.2) in solving the model problem is analyzed. From the stability analysis, parameters influencing the stability of the algorithm are identified and the equation
for the amplification factor based on the parameters is obtained. The analysis is further used to demonstrate that the partitioned algorithm is unstable for large Fourier numbers, unlike the monolithic approach. Accordingly, a stability criterion is obtained.

Following Giles [11] (in which stability is analyzed using Backward Euler for time integration), the stability theory of Godunov and Ryabenki is used to analyze the stability of this partitioned algorithm. In order to simplify the analysis, the explicit corrector step will not be incorporated into the stability analysis. However, in the results section, the stability of the algorithm is investigated numerically with the explicit corrector step incorporated, and the results are compared to the analytical stability analysis.

The one-dimensional model problem described in section 2.2 is used for the stability analysis, with the modification that the two coupled domains are considered to be semi-infinite. The non-interface boundary conditions \((x \to \pm \infty)\) are then given by:

\[
T_1(x \to -\infty, t) = T_{1,lbc}, \quad (4.31)
\]

\[
T_2(x \to \infty, t) = T_{2,rbc}. \quad (4.32)
\]

Our point of departure is the semi-discretization of each subdomain:

\[
(\Delta x \rho c_p)_{1} \frac{dT_{1,j}}{dt} = F_{1,j} = \frac{k_1}{\Delta x_1} (T_{1,j-1} - 2T_{1,j} + T_{1,j+1}) \quad j < 0, \quad (4.33)
\]

\[
(\Delta x \rho c_p)_{1} \frac{dT_{1,0}}{dt} = F_{1,0} = -q_{1,0} - \frac{k_1}{\Delta x_1} (T_{1,0} - T_{1,-1}), \quad (4.34)
\]

\[
(\Delta x \rho c_p)_{2} \frac{dT_{2,j}}{dt} = F_{2,j} = \frac{k_2}{\Delta x_2} (T_{2,j-1} - 2T_{2,j} + T_{2,j+1}) \quad j > 0, \quad (4.35)
\]

where the spatial operators in the governing equations have been discretized and the interface conditions are given by (4.7)-(4.8). The \(\theta\) scheme is applied to discretize the time derivative in (4.33)-(4.35). The resultant implicit system is solved approximately using the loosely-coupled partitioned algorithm. While in the monolithic method, both the interface equations are treated implicitly ((4.13)-(4.14)), this is not the case in a partitioned algorithm. Here, the subdomain \(\Omega_1\), to which the flux condition is assigned at the interface, is integrated first (BGS-12). Hence, it follows that the continuity of temperature at the interface is satisfied at every time-step. In the discretization of \(T_{1,0}^{n+1}\), the interface heat flux at \(t^{n+1}\), \(q_{1,0}^{n+1}\), is predicted using the previous time step solution of \(q_{2,0}^{n}\):

\[
\tilde{q}_{1,0} = q_{2,0}^{n} = -\frac{k_2}{\Delta x_2} (T_{2,1}^{n} - T_{2,0}^{n}). \quad (4.36)
\]

As Algorithm 1 shows, the interface terms are updated at the end of each time-level. As a result, in the discretization of \(T_{1,0}^{n+1}\), the interface flux \(q_{1,0}^{n}\) in \(F_1^n\) is equal to
\[ q_{2,0}^n = q_{1,0}^n = -\frac{k_2}{\Delta x_2} (T_{2,1}^n - T_{2,0}^n). \]  

(4.37)

Taking the above considerations into account, the following system of equations for the loosely-coupled partitioned algorithm where \( \Omega_1 \) is integrated first is obtained:

\[
T_{1,j}^{n+1} = T_{1,j}^n + \theta d_1 (T_{1,j-1} - 2T_{1,j} + T_{1,j+1})^n + (1 - \theta) d_1 (T_{1,j-1} - 2T_{1,j} + T_{1,j+1})^n \quad j < 0, \\
T_{1,0}^{n+1} = T_{1,0}^n - 2\theta d_1 (T_{1,0} - T_{1,-1})^n + 2\theta d_2 (T_{2,1} - T_{2,0})^n, \\
T_{2,j}^{n+1} = T_{2,j}^n + \theta d_2 (T_{2,j-1} - 2T_{2,j} + T_{2,j+1})^n + (1 - \theta) d_2 (T_{2,j-1} - 2T_{2,j} + T_{2,j+1})^n \quad j > 0, \\
T_{2,0}^{n+1} = T_{1,0}^{n+1}, \\
T_{2,0}^n = T_{1,0}^n.
\]

(4.38)

where \( r \) is defined by:

\[
r = \left( \frac{\rho c_p \Delta x}{\rho c_p \Delta x} \right)^2.
\]

(4.39)

and \( d_m \) (the Fourier number of \( \Omega_m \)) by:

\[
d_m = \Delta t_k_m \frac{\Delta t_{\alpha_m}}{\rho c_p \Delta x_m^2} = \frac{\Delta t_{\alpha_m}}{\Delta x_m^2}.
\]

(4.40)

Noting that the model problem is not periodic, the von Neumann stability analysis cannot be applied. Following Giles \[11\], the stability theory of Godunov and Ryabenkii is considered. In this approach, the existence of separable normal modes of the form,

\[
T_j^n = z^n \kappa^j
\]

(4.41)
is examined, where \( \kappa \) is the space amplification factor (\( \kappa^j \) represents the spatial modes) and \( z \) the time-amplification factor [37]. For the far field boundary conditions to be satisfied (\( \kappa^j \to 0 \) as \( j \to \pm \infty \)), it is required that \( |\kappa| < 1 \). The discretization (4.38) is unstable, if the difference equations admit such form of solutions which satisfy the far field boundary conditions and have \( |z| > 1 \), resulting in exponential growth in time. The form of the solution is quite similar to the Fourier modes assumed in the von Neumann stability analysis, except that the amplitude of the spatial oscillations decay exponentially with \( |j| \) away from the interface. \[11\]

For this partitioned algorithm, the form of the normal mode solution is given by:

\[
T_{m,j}^n = z^n \kappa_m^j = \begin{cases} 
  z^n \kappa_1^j & m = 1, j \leq 0, \\
  z^n \kappa_2^j & m = 2, j \geq 0
\end{cases}
\]

(4.42)
4.4. Stability analysis

where the two last equations in (4.38) are satisfied as a result of the selected normal modes. The other equations in (4.38) require that the variables \( z, \kappa_1 \) and \( \kappa_2 \) satisfy the equations:

\[
\begin{align*}
1 &= z^{-1} + d_1(\kappa_1 - 2 + \kappa_1^{-1})(\theta + (1 - \theta)z^{-1}) , \\
1 &= z^{-1} + 2d_1(-1 + \kappa_1^{-1})(\theta + z^{-1}(1 - \theta)) + 2rd_2z^{-1}(\kappa_2 - 1) , \\
1 &= z^{-1} + d_2(\kappa_2 - 2 + \kappa_2^{-1})(\theta + (1 - \theta)z^{-1}) .
\end{align*}
\]

(4.43)

Solving the first and last equations for \( \kappa_1^{-1} \) and \( \kappa_2 \), we obtain:

\[
\begin{align*}
\kappa_1^{-1} &= 1 + \frac{1 - z^{-1}}{2d_1(\theta(1 - z^{-1}) + z^{-1})} \left[ 1 \pm \sqrt{1 + \frac{4d_1(\theta(1 - z^{-1}) + z^{-1})}{1 - z^{-1}}} \right] , \\
\kappa_2 &= 1 + \frac{1 - z^{-1}}{2d_2(\theta(1 - z^{-1}) + z^{-1})} \left[ 1 \pm \sqrt{1 + \frac{4d_2(\theta(1 - z^{-1}) + z^{-1})}{1 - z^{-1}}} \right] .
\end{align*}
\]

(4.44)

In order to satisfy the far field boundary conditions, we must have \(|\kappa_1^{-1}| < 1 \) and \(|\kappa_2| < 1 \). Thus, for the case of real and positive arguments within the square-roots, the negative roots must be selected. Substituting the two into the second equation in (4.43), we obtain the equation for the amplification factor, i.e. \( z \):

\[
\sqrt{1 + \frac{4d_1(\theta(1 - z^{-1}) + z^{-1})}{1 - z^{-1}}} + \frac{rz^{-1}}{\theta(1 - z^{-1}) + z^{-1}} \left[ \sqrt{1 + \frac{4d_2(\theta(1 - z^{-1}) + z^{-1})}{1 - z^{-1}}} - 1 \right] = 0.
\]

(4.45)

Since obtaining a closed form solution to \( z \) is not trivial, usually asymptotic solutions are considered under certain assumptions.

When the model problem is solved monolithically with the \( \theta \) scheme \((0.5 \leq \theta \leq 1)\) for time integration, the solution algorithm is unconditionally stable. Of interest is to analyze whether same holds true (unconditionally stability) using the partitioned algorithm. Therefore, under the assumption of \( d_m \gg 1 \), (4.45) reduces to:

\[
\sqrt{d_1} + \frac{rz^{-1}}{\theta(1 - z^{-1}) + z^{-1}} \sqrt{d_2} \approx 0,
\]

(4.46)

with the asymptotic solution given by:

\[
z \approx 1 - \frac{1}{\theta}(1 + \sqrt{\frac{d_2}{d_1}}r).
\]

(4.47)
For stability $|z| < 1$ and therefore, $0 < \frac{1}{\theta}(1 + \sqrt{\frac{d_2}{d_1}} r) < 2$. Using the definitions of $d_1$, $d_2$, and $r$, the obtained stability criterion can also be written as $0 < \frac{1}{\theta}(1 + \sigma) < 2$ with $\sigma$ defined in (2.28). Based on the discussion in section 3.1, $0 < \sigma < 1$. Therefore, the algorithm is unstable for $\theta = 0.5$ (Crank-Nicolson). For Backward Euler, the criterion reduces to $\sigma < 1$ which is true by the correct assignment of the interface boundary conditions. This implies that Backward Euler should retain its stability for large Fourier numbers; a similar conclusion was obtained in [11] for Block Jacobi.

Since the loosely-coupled algorithm with $\theta = 0.5$ is unstable for $d_m \gg 1$, it is of interest to obtain the point at which instability initiates. Following [37], first (4.45) is solved for $r$:

$$r = -\frac{\theta(1 - z^{-1}) + z^{-1}}{z^{-1} \left[ 1 + \frac{4d_1(\theta(1-z^{-1})+z^{-1})}{1-z^{-1}} - 1 \right]}.$$  \hspace{1cm} (4.48)

Instability initiates when $|z| = 1$. Noting that $r$ is real (based on its definition (4.39)), from (4.48) it follows that $z$ must be real as well. Substituting $z = 1$ into (4.48) yields $r = -\sqrt{\frac{d_2}{d_1}}$ which is not possible noting that $r$ is positive. Therefore, by substituting $z = -1$ into (4.48), the value of $r$ at which instability initiates is obtained:

$$r_s = \frac{(2\theta - 1)\sqrt{1 + 2d_1(2\theta - 1)}}{1 + \sqrt{1 + 2d_2(2\theta - 1)}}.$$  \hspace{1cm} (4.49)

It is observed that $r_s(\theta = 0.5)$ is not defined. Using l’Hospital’s Rule to evaluate the limit, we arrive at:

$$\lim_{\theta \to 0.5} r_s(\theta) = \frac{1}{d_2}.$$  \hspace{1cm} (4.50)

Therefore, when $\theta = 0.5$, for stability $rd_2 < 1$. By substituting the definitions of $r$ and $d_2$ into the criterion, we obtain that

$$\frac{\Delta t}{\Delta x_1 \Delta x_2} < 1,$$  \hspace{1cm} (4.51)

which imposes restriction on $\Delta t$ given the material properties and grid size of the coupled domains.

By removing steps 3 and 5 of Algorithm 1, a different loosely-coupled solution algorithm (see Algorithm 2) can be defined in which the solution at the end of the predictor step in Algorithm 1 is taken as the time step solution. Furthermore, the interface conditions are not updated at the end of the time-step. In Appendix A, stability analysis is performed for this loosely-coupled algorithm.

The asymptotic solution for the amplification factor for the case of $d_m \gg 1$ is given by $z \approx -\sqrt{\frac{d_2}{d_1}} r = -\sigma$, which is independent of $\theta$. Therefore, the algorithm
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**Algorithm 2** Pseudocode of a loosely-coupled algorithm; using BGS-12

1: Assign $q_{1,n}^n$ to $\Omega_1$ and solve for $T_1^n$, (4.15).
2: Assign $T_{2,n}^n$ to $\Omega_2$ and solve for $T_2^n$, (4.16).
3: Compute residual vector $F_1^*(T_1^n, q_{1,n}^n, I^n, t^{n+1})$ and $F_2^*(T_2^n, T_{2,n}^n, I^n, t^{n+1})$, (4.9)–(4.10).

should retain its stability when $d_m \gg 1$ by the correct assignment of the interface boundary conditions. However, in the section on accuracy analysis, it was observed that the solution at the end of the predictor step suffers order reduction for $\theta = 0.5$. Therefore, the partitioned algorithm given by Algorithm 2 does not preserve the time integration’s design order.

It is noted that in practice, for 2-D and 3-D computations, while satisfying the stability criteria obtained for this 1-D model problem is necessary, they may or may not be sufficient ones [11].

4.4.1 Numerical results

In the stability analysis, the corrector step was omitted from the analysis. But noting that we are interested in preserving the time integration order, the stability of the algorithm is investigated numerically (using the 1-D model problem) with the explicit corrector step incorporated.

The following parameters are used for the 1-D test case. Each subdomain has a length of $L_m = 0.5$ and is discretized using VFV method with $N_m = 500$ ($N_m$: number of nodes in $\Omega_m$, the mesh is uniform). The following initial condition is imposed on the global domain: $T(x, t = 0) = 0, x \in \Omega_1$ and $T(x, t = 0) = 1, x \in \Omega_2$. The non-interface boundary conditions are set to $T_1(x = -0.5, t) = 0$ and $T_2(x = 0.5, t) = 1$. The materials of the coupled domains are varied according to Table 4.2 (see Table 4.1 for specifications of the material properties). The Crank-Nicolson scheme $\theta = 0.5$ is used for time-integration. The coupled problem is solved by integrating $\Omega_1$ first (BGS-12) (similar results are obtained using BGS-21). For each case, $\Delta t$ is incremented until the computations become unstable. The approximate $\Delta t$ and $d_m$ at which simulations become unstable are presented in Table 4.2.

<table>
<thead>
<tr>
<th>Material</th>
<th>$\rho \ [kg/m^3]$</th>
<th>$c_p \ [J/kg\cdot K]$</th>
<th>$k \ [W/m\cdot K]$</th>
<th>$\alpha \ [m^2/s]$</th>
<th>$e \ [W/(m\cdot K)^2]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steel</td>
<td>$7.5 \cdot 10^3$</td>
<td>$5.0 \cdot 10^2$</td>
<td>$4.8 \cdot 10^4$</td>
<td>$1.3 \cdot 10^{-5}$</td>
<td>$1.3 \cdot 10^4$</td>
</tr>
<tr>
<td>Water</td>
<td>$1.0 \cdot 10^3$</td>
<td>$4.2 \cdot 10^3$</td>
<td>$6.0 \cdot 10^{-1}$</td>
<td>$1.4 \cdot 10^{-7}$</td>
<td>$1.6 \cdot 10^3$</td>
</tr>
<tr>
<td>Air</td>
<td>$1.0 \cdot 10^0$</td>
<td>$1.0 \cdot 10^3$</td>
<td>$3.0 \cdot 10^{-2}$</td>
<td>$3.0 \cdot 10^{-5}$</td>
<td>$5.5 \cdot 10^0$</td>
</tr>
</tbody>
</table>

For $\theta = 0.5$, it was derived (excluding the corrector step) that for stability $r d_2 < 1$. For all the three cases in Table 4.2, it is observed that instability initiates...
Table 4.2: Stability of the loosely-coupled algorithm with Crank-Nicolson for time integration.

<table>
<thead>
<tr>
<th>case</th>
<th>$\sigma$</th>
<th>$r$</th>
<th>$d_1$</th>
<th>$d_2$</th>
<th>$\Delta t$</th>
<th>$rd_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>steel-air</td>
<td>$4.1 \cdot 10^{-4}$</td>
<td>$2.7 \cdot 10^{-4}$</td>
<td>$1.6 \cdot 10^3$</td>
<td>$3.8 \cdot 10^3$</td>
<td>$1.3 \cdot 10^2$</td>
<td>$1.0016$</td>
</tr>
<tr>
<td>steel-water</td>
<td>$1.2 \cdot 10^{-1}$</td>
<td>$1.1 \cdot 10^0$</td>
<td>$8.0 \cdot 10^1$</td>
<td>$8.9 \cdot 10^{-1}$</td>
<td>$6.3 \cdot 10^0$</td>
<td>$1.0016$</td>
</tr>
<tr>
<td>steel-steel</td>
<td>$1 \cdot 10^0$</td>
<td>$1 \cdot 10^0$</td>
<td>$1.0 \cdot 10^0$</td>
<td>$1.0 \cdot 10^0$</td>
<td>$7.8 \cdot 10^{-2}$</td>
<td>$1.0001$</td>
</tr>
</tbody>
</table>

when this criterion is not satisfied. Therefore, (4.50) also provides a good estimate of the stability limit when the explicit corrector step is incorporated into the scheme. The stability of the coupling algorithm using two and three corrector steps was also investigated. The approximate $\Delta t$ at which the simulation becomes unstable is $\Delta t = 2.2$ and $\Delta t = 0.6$ for two and three corrector steps respectively. As the results indicate, by performing more (explicit) corrector steps, the stability region of the algorithm reduces.

For the case of steel-air coupling, it is observed that instability initiates at large Fourier numbers of the domains relative to the other two cases. Based on the stability criterion obtained for $\theta = 0.5$ ($rd_2 < 1$), when $r \ll 1$, it follows that $d_2$ can take large values ($d_2 \gg 1$) while still adhering to the criterion. Inversely, when $r \gg 1$, it follows that $d_2 \ll 1$ in order to satisfy the criterion.

For each considered case, the corresponding value of $\sigma$, defined in (2.28), has also been included in the table. As the results in the table demonstrate, the loosely-coupled algorithm performs better when the thermal interaction between the coupled domains is weak, $\sigma \ll 1$, compared to cases where the thermal interaction is strong, $\sigma \rightarrow 1$.

In the later chapters, the cell centered finite volume CFV is used to discretize the subdomains. Therefore, in order to investigate the influence of the spatial discretisation using CFV on the stability of the loosely coupled algorithm, the same 1–D test case is considered. Noting that $\Omega_1$ does not have a node at the interface as a result of the cell-centered discretization, linear extrapolation from the cells in $\Omega_1$ close to the interface is used to approximate the interface temperature (see section 3.2 for more details). The length of each subdomain is $L_m = 0.5$ and is divided into $N_m = 500$ finite volumes of equal size ($\Delta x_m = 1 \cdot 10^{-3}$). Again, the Crank-Nicolson scheme is used for time integration. The results using the BGS-12 sequence are shown in Table 4.3 (similar results are obtained using BGS-21).

Based on the results in the table, an estimate of the stability criterion appears to be

$$rd_2 < \frac{1}{\xi}. \quad (4.52)$$

with $\xi = 3/2$. By substituting the definitions of $r$ and $d_2$ into the criterion, we
Table 4.3: Stability of the loosely-coupled algorithm using CFV for spatial discretisation.

<table>
<thead>
<tr>
<th>case</th>
<th>σ</th>
<th>r</th>
<th>$d_1$</th>
<th>$d_2$</th>
<th>$\Delta t$</th>
<th>$rd_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>steel-air</td>
<td>$5.8 \cdot 10^{-4}$</td>
<td>$2.7 \cdot 10^{-4}$</td>
<td>$5.4 \cdot 10^2$</td>
<td>$2.5 \cdot 10^3$</td>
<td>$4.2 \cdot 10^1$</td>
<td>0.672</td>
</tr>
<tr>
<td>steel-water</td>
<td>$1.3 \cdot 10^{-1}$</td>
<td>$1.3 \cdot 10^0$</td>
<td>$5.4 \cdot 10^1$</td>
<td>$5.3 \cdot 10^{-1}$</td>
<td>$4.2 \cdot 10^0$</td>
<td>0.672</td>
</tr>
<tr>
<td>steel-steel</td>
<td>$1 \cdot 10^0$</td>
<td>$1 \cdot 10^0$</td>
<td>$6.7 \cdot 10^{-1}$</td>
<td>$6.7 \cdot 10^{-1}$</td>
<td>$5.2 \cdot 10^{-2}$</td>
<td>0.667</td>
</tr>
</tbody>
</table>

obtain that:

$$\frac{\Delta t \frac{k_c}{(\rho c_p)_L}}{\Delta x_1 \Delta x_2} < \frac{1}{\xi},$$

(4.53)

which imposes restriction on $\Delta t$ given the material properties and grid size of the coupled domains (compare this criterion to $rd_2 < 1$ obtained for VFV discretization).

It is noted in (3.7) that $\xi$ is one of the parameters that appears in the equation to obtain the interface temperature using linear extrapolation.

4.5 Numerical Example

In this section an unsteady conjugate heat transfer problem is considered (the fluid domain is modeled using the Boussinesq approximation of the Navier-Stokes system and the solid domain using heat conduction -see Chapter 2). The loosely coupled partitioned algorithm presented in section 4.2 is applied to solve the problem in order to demonstrate the applicability of the method and its order preservation.

4.5.1 Problem description and specifications

As a test-case, unsteady conjugate natural convection in a square enclosure is considered. The configurations of the problem, shown in Fig. 4.2, follows from Kaminski and Prakash [20] where the steady-state solution of the coupled problem was sought. The solid domain occupies the rectangular region $\Omega_1 = [0,L] \times [-h,0]$ and the fluid domain occupies the square region $\Omega_2 = [0,L] \times [0,L]$ with the interface between the two domains located at $I = [0,L] \times 0$. The vertical boundaries (at $x = 0$, and $x = L$) of both the solid and fluid domains are insulated. Dirichlet conditions are prescribed to the top boundary of the fluid domain ($T(x,L) = T_C$) and the lower boundary of the solid domain ($T(x,-h) = T_{Hi}$). The gravity acts in the $-x$ direction ($j = (-1,0,0)$).
The test-case is solved using the following parameters of the problem:

$$\begin{align*}
k_1 &= 1600, \quad \rho_1 = 7500, \quad c_{p,1} = 0.5, \\
k_2 &= 1, \quad \rho_2 = 1, \quad c_{p,2} = 1, \quad \nu_2 = 0.7, \quad \beta = 0.01, \quad g = 0.7 \cdot 10^7, \\
L &= 1, \quad h = 0.2, \quad T_{ref} = 1, \quad T_H = 2, \quad T_C = 1, \\
k_1 k_2 &= 1600, \quad \frac{\kappa_1}{\kappa_2} = 0.4, \quad Pr = 0.7, \quad Ra = 1 \cdot 10^5,
\end{align*}$$

The ratio between the material properties of the coupled domains in (4.54) correspond to those of steel and air. Therefore, the thermal interaction between the coupled domains is weak ($\sigma = 4.1 \cdot 10^{-4} \ll 1$). Based on the prescribed values of the material properties, for stability $\Omega_2$ takes the Dirichlet condition at the interface, while $\Omega_1$ the Neumann condition.

### 4.5.2 Solution procedure

The solid domain $\Omega_1$ is discretized using the finite volume method with the temperature stored in the cell center. The fluid domain $\Omega_2$ is also discretized using the finite volume method with staggered arrangement of the variables [44]. In each of the subdomains, a uniform grid-spacing is used in both directions: for the solid domain: $N_{1,x} = 80, N_{1,y} = 20$ with $N$ number of cells, and for the fluid domain $N_{2,x} = 80, N_{2,y} = 80$. Noting that $\Omega_1$ does not have a node at the interface as result of the cell-centered discretization, linear extrapolation from the cells in $\Omega_1$ close to the interface is used to approximate the interface temperature (see section 3.2 for more details). In both the momentum and energy equations, the second order centered scheme is used for discretizing the convective terms and the second order differencing scheme is used to discretize the diffusive terms. The Crank-Nicolson
scheme is used for time integration. In the flow solver, at each time level, Picard iterations are used for solving the non-linear coupled equations [44]. The flow solver is iterated to a strict tolerance ($\epsilon_{\text{iter}} < 10^{-9}$, $\epsilon_{\text{iter}}$: maximum of the residuals of the momentum and energy equations) to eliminate iteration error as a contaminating variable in the study.

Initially, the global domain is set to a temperature of unity: $T(x,t = 0) = 1$ for $x \in \Omega = \Omega_1 \cup \Omega_2$. Then, computations are carried out using the monolithic approach (also with Crank-Nicolson for time integration) to $t = 0.01$ using a time step of $\Delta t = 10^{-5}$, in order to step over the time that is required for the heat to travel from the bottom boundary to the interface (thermal interaction between the two subdomains has been initiated at this time). The obtained solution at $t = 0.01$ is used as initial condition for the problem.

The coupled problem is advanced in time to $t_{\text{final}} = 0.06$ using the loosely-coupled algorithm with various time-step values. The partitioned solution at $t_{\text{final}}$ was compared to that of the temporally exact solution (the monolithic solution at $t_{\text{final}}$ obtained using a fine time step of $\Delta t = 10^{-5}$). To investigate how well the coupled problem is solved compared to the monolithic approach, computations are also carried out with the monolithic solver.

### 4.5.3 Temporal accuracy

The time integration error ($\epsilon_{\text{t}}$) is defined as the difference between the temporally exact solution and the monolithic solution at $t_{\text{final}}$ obtained with a certain time step which is coarser relative to $\Delta t_{\text{fine}}$. The difference between the temporally exact solution and the partitioned solution at $t_{\text{final}}$ is defined as the total error in the partitioned solution ($\epsilon_{\text{total}}$) and represents the sum of the time integration error ($\epsilon_{\text{t}}$) and partitioning error ($\epsilon$), ($\epsilon_{\text{total}} = \epsilon_{\text{t}} + \epsilon$). For $\epsilon_{\text{total}}$ to be of the same order as $\epsilon_{\text{t}}$, the partitioning error $\epsilon$ needs to be at least of the same order as $\epsilon_{\text{t}}$. In Fig. 4.3, the total error in the global temperature field obtained with the loosely-coupled algorithm is shown as a function of time step size. Also shown, is the corresponding (time integration) error in temperature field obtained using the monolithic approach.

As Fig. 4.3a shows, when the solution at $t^{n+1}$ is approximated by the solution to the predictor step ($T^{m}_m$) (denoted in the figure by $BGS-21,\text{pred}$), the partitioned solution suffers from order reduction. This is in accordance with the one-step error analysis. By updating the interface terms and performing one explicit corrector step ($T^{m*}_m$), the temporal order of accuracy of the partitioned solution (denoted in the figure by $BGS-21$) is retrieved as the one-step analysis also demonstrated. Therefore, to preserve the time integration order, the need to perform an additional implicit solve (a subiteration) at each time-step is avoided. As shown in Fig. 4.3a, this holds irrespective of the sequence with which the domains are solved.

For a time accurate partitioned solution, the level of the partitioning error should be as low as possible, desirably below the time integration error such that the partitioning is not the dominant source of error in the partitioned solution. In Fig. 4.3a,
by comparing the total error in the temperature field obtained with the two different integration sequences with the corresponding (time integration) error in the monolithic solution, it is observed that the partitioned solution obtained by integrating $\Omega_1$ first (BGS-12) is more accurate than the partitioned solution obtained using BGS-21 and for this test-case is as accurate as the monolithic solution. By examining the solution to the coupled problem obtained using BGS-21 and comparing it to that of the monolithic solution (see Fig. 4.3b), a temperature discontinuity at the interface between the two domains is observed, along with temperature under and overshoots in the fluid cells next to the interface. As the time step size decreases, the magnitude of such discrepancies between the monolithic and the partitioned solution reduce and vice-versa as evident in the variation of the level of total error with $\Delta t$.

In solving the coupled problem using BGS-21, the partitioning error (as a result of segregated solve of the interface equations) is placed entirely in the continuity of the interface temperature equation and therefore this equation is solved approximately while the continuity of the interface heat flux is satisfied exactly. This is in opposite to solving the problem using BGS-12. In general it is not clear which approximation (having a discontinuity in the interface heat flux or interface temperature) is less disadvantageous and seems to be an issue which is problem dependent. At least for this test case, as the results in Fig. 4.3a demonstrate, using BGS-12 provides a solution which is more accurate than BGS-21.

4.5.4 Stability

For the CHT problem considered in this section, noting that CFV is used to discretize the subdomains, substituting the model parameters into (4.52), the estimated $\Delta t$
at which instabilities initiate is $\Delta t = 0.3125$. By performing computations using $\Delta t = 0.3$ and $\Delta t = 0.32$, it is observed that while the solution algorithm is stable for the first time step size, it is unstable for the latter. Therefore, the obtained analytical criteria, provides a good estimate of the point at which the coupling algorithm becomes unstable.

4.6 Conclusions

A second-order time-accurate loosely-coupled partitioned algorithm was presented for solving transient thermal coupling of solids and fluids, or conjugate heat transfer (CHT). The Crank-Nicolson scheme is used to advance the solution within each separate fluid and solid subdomains. The accuracy and stability of the loosely-coupled solution algorithm were analyzed.

Based on the accuracy analysis, the design order of the time integration scheme is preserved by following a predictor (implicit)-corrector (explicit) approach at each time-step. Therefore, the need to perform an additional implicit solve (a subiteration) at each time-step is avoided. The analytical stability analysis shows that by using the Crank-Nicolson scheme for time integration, the partitioned algorithm is unstable for large Fourier numbers, unlike the monolithic approach. This is also in contrast to the unconditional stability of the partitioned algorithm with Backward Euler for time integration. Accordingly, using the stability analysis, a stability criterion is obtained for the Crank-Nicolson scheme that imposes restriction on $\Delta t$ given the material properties and mesh spacings of the coupled domains ($\frac{\Delta t}{\Delta x_1^2 \rho c_p} < 1$). Numerical examples were used to demonstrate the applicability of the algorithm.
Chapter 5

High order IMEX schemes and a loosely-coupled solution algorithm


As demonstrated in the previous chapter, loosely-coupled solution algorithms can provide an efficient way of solving time-accurate weakly-coupled CHT problems relative to the monolithic approach. Yet, obtaining time-accurate solutions can remain computationally expensive (due to the use of a low order time integration scheme). As a potential solution, in this chapter a loosely-coupled solution algorithm is presented in which the high order IMEX schemes discussed in Chapter 3 are used for time integration. The IMEX schemes consist of the ESDIRK schemes which are used for advancing the solution in time within each separate fluid and solid subdomain and equal order and number of stages ERK schemes for explicit integration of part of the coupling terms.

Using the results of the analysis for Crank-Nicolson as reference, the temporal order of accuracy and stability of the loosely coupled algorithm in which the IMEX schemes are used for time integration will be investigated by considering some numerical experiments. We investigate whether the temporal design order of the high order ESDIRK schemes employed within each separate subdomain is preserved for the coupled simulations (without subiterating). In addition, whether a condition which will indicate the possibility of using large Fourier number of subdomains can be obtained.

While in the loosely coupled multi-stage IMEX schemes a single interface iteration is performed at each (implicit) stage, in the second order loosely coupled
Crank-Nicolson scheme, only one is performed per time-step. However, for the same time-step, the high order IMEX schemes generally provide temporally more accurate solutions. For a CHT test-case, the (computational) work-(temporal) precision character of the high order IMEX and second order Crank-Nicolson and BDF2 schemes is compared over a range of accuracy requirements. We investigate whether the high order IMEX schemes can compete with the second order schemes for a reasonable portion of the work-precision spectrum, i.e. whether the additional work per time-step of the IMEX schemes is compensated by the gain in temporal accuracy.

5.1 Solution Algorithm

In this section, the details of the loosely-coupled solution algorithm is presented where the IMEX schemes (discussed in section 3.4) are used for time integration.

We consider solving the coupled system at each stage, integrating $\Omega_2$ first, i.e. using Block Gauss-Seidel (BGS-21).

In computing the temperature field in $\Omega_2$ at an implicit stage of the ESDIRK schemes (the semi-discretized form of $T_2$ is given in (3.4)-(3.6)), the coupling term $f_{21} = \frac{k_2}{\Delta x_{2,b}} T_{2,1}$ is treated explicitly and integrated with the ERK schemes. In other words, the semi-discrete form of $T_2$ is integrated in time using the IMEX schemes:

$$M_2(T_2^{(k)} - T_2^n) = \Delta t \sum_{i=1}^{k} a_{ki}^E \left( A_2 T_2^{(i)} + f_2^{(i)} \right) + \Delta t \sum_{i=1}^{k-1} a_{ki}^E \left( f_2^{(i)} b_2 \right),$$

(5.1)

where $A_2$ represents the discretization of the diffusion term, and $f_2$ is a vector containing the contribution of the non-interface boundary. The vector $b_2$ contains zero entries except for the discretization of the cell next to the interface, $T_{2,1}$, for which its entry is 1. Integrating the coupling term using the ERK schemes, is equivalent to using the following flux predictor:

$$f_{21}^{(s)} = \sum_{i=1}^{k-1} a_{ki}^E - a_{ki}^I f_{21}^{(i)} ,$$

(5.2)

in computing the stage solution $T_2^{(k)}$:

$$M_2(T_2^{(k)} - T_2^n) = \Delta t a_{kk}^l \left( A_2 T_2^{(k)} + f_{21}^{(s)} b_2 + f_2^{(k)} \right) + \Delta t \sum_{i=1}^{k-1} a_{ki}^I \mathcal{F}_2^{(i)},$$

(5.3)

where $\mathcal{F}_2^{(i)}$ is the residual vector of any of the stages defined by:

$$\mathcal{F}_2^{(i)} = A_2 T_2^{(i)} + f_{21}^{(i)} b_2 + f_2^{(i)}.$$

(5.4)

The equivalence between (5.1) and (5.3) can be readily observed by substituting (5.2) into (5.3).
5.1. Solution Algorithm

When the thermal conductivity and the mesh is fixed in time, the coefficient \( \frac{k_2}{Ax_{2,b}} \) in \( f_{21} = \frac{k_2}{Ax_{2,b}} T_{2,1} \) is constant and therefore the flux-predictor in (5.2) is reduced to predicting the interface temperature (i.e. state-predictor):

\[
T_{2,1}^{(s)} = \sum_{i=1}^{k-1} \frac{q_{ki}}{a_{ki}} T_{2,i}^{(i)},
\]

(5.5)

With \( T_{2}^{(k)} \) computed, we assign:

\[
q_{1,1}^{(s)} = q_{2,1}^{(s)} = -\frac{k_2}{Ax_{2,b}} (T_{2,1}^{(k)} - T_{2,1}^{(s)})
\]

(5.6)

and solve for \( T_{1}^{(k)} \) using the ESDIRK schemes:

\[
M_1(T_{1}^{(k)} - T_{1}^{(s)}) = \Delta t a_{kk} \left( A_1 T_{1}^{(k)} - q_{1,1}^{(i)} b_1 + f_{1}^{(i)} \right) + \Delta t \sum_{i=1}^{k-1} a_{ki} \mathcal{F}_{1}^{(i)},
\]

(5.7)

where \( A_1 \) represents the discretization of the diffusion term, and \( f_{1} \) is a vector containing the contribution of the non-interface boundary. The vector \( b_1 \) contains zero entries except for the discretization of the cell next to the interface for which its entry is 1. \( \mathcal{F}_{1}^{(i)} \) is the residual vector of any of the stages:

\[
\mathcal{F}_{1}^{(i)} = A_1 T_{1}^{(i)} - q_{1,1}^{(i)} b_1 + f_{1}^{(i)}
\]

(5.8)

With the stage temperature field \( T_{m}^{(k)} \) computed, the interface conditions are updated:

\[
T_{1,1}^{(k)} = \mu T_{1,-2}^{(k)} + \zeta T_{1,-1}^{(k)}
\]

(5.9)

\[
T_{2,1}^{(k)} = T_{2,1}^{(k)}
\]

(5.10)

\[
q_{2,1}^{(k)} = -\frac{k_2}{Ax_{2,b}} (T_{2,1}^{(k)} - T_{2,1}^{(k)})
\]

(5.11)

\[
q_{1,1}^{(k)} = q_{2,1}^{(k)}
\]

(5.12)

and the stage residual vectors \( \mathcal{F}_{1}^{(k)} \) and \( \mathcal{F}_{2}^{(k)} \) are computed using (5.8) and (5.4) respectively.

After solving all \( s \) stages, the solution to the time-level \( T_{m+1}^{n+1} \) is obtained by using (3.15) where through cancelation of the lower order error terms, \( T_{m+1}^{n+1} \) has the designed high order accuracy.

The solution procedure is the same when the coupled problem is solved by integrating \( \Omega_1 \) first (BGS-12). In solving for the temperature field in \( \Omega_1 \), a prediction of the flux at the interface is required which is given by (5.5), with \( T_{2,1} \) replaced with \( q_{1,1} \). After solving for \( T_1 \), the interface temperature is evaluated using (3.7) and is imposed as the interface condition on \( \Omega_2 \).
5.1.1 Stability of the solution algorithm

Because of partitioning, there is the possibility of numerical instability not inherent in the monolithic approach [11]. In the previous chapter, by applying the stability theory of Godunov and Ryabenkii, the stability of the loosely coupled solution algorithm with the $\theta$ scheme for time integration was analyzed. For stable computations using the predictor-corrector Crank-Nicolson scheme, the criterion,

$$rd_2 < \gamma \Rightarrow \frac{\Delta t \frac{k_T}{\rho c_p}}{\Delta x_1 \Delta x_2} \frac{1}{\sigma} \frac{1}{\Delta x_1 \Delta x_2} < \gamma,$$  \hfill (5.13)

needs to be satisfied, where $\gamma$ is equal 1 for the vertex-based discretization and $2/3$ for the cell-center discretization with linear extrapolation of the interface temperature. The stability criterion can also be expressed in the following useful form:

$$\sigma \sqrt{d_1 d_2} < \gamma,$$  \hfill (5.14)

which directly relates the strength of the coupling $\sigma$ to the stability of the algorithm.

Applying the same stability theory to the IMEX schemes is not straightforward, given the multiple stages (Butcher tableau coefficients). However, it is possible to identify parameters that may influence the stability of the coupling algorithm based on the fully-discretized equations. For the purpose of analysis, it is more convenient to cast the system of difference equations (for a stage) of the loosely-coupled IMEX into the form shown in Appendix B. The equations, correspond to integrating $\Omega_1$ first (BGS-12). It is noted that in the discretization of the interface node $T_{1,0}$, \hfill (B.2), the product $\sigma \sqrt{d_1 d_2}$ is part of the coupling term. Furthermore, for the predictor-corrector Crank-Nicolson, as shown earlier, the product also appears in the stability criterion (5.14). Hence, it can be expected that this product is an influential parameter in the stability of the high order IMEX schemes. This issue will be further investigated in the results section.

5.2 Numerical Examples

In this section, the loosely coupled solution algorithm presented in section 5.1 is used to solve a conjugate heat transfer problem in order to demonstrate the applicability of the algorithm, to investigate the temporal order preservation and stability of the algorithm, and finally its computational efficiency relative to commonly used 2nd order time integration schemes. Initially results are shown for a case with constant material properties. This is followed by investigating the temporal order of the IMEX schemes when the thermal conductivities are temperature dependent.

5.2.1 Problem description and specifications

As a test-case, the unsteady conjugate natural convection in a square enclosure presented in section 4.5 is considered. The accuracy and stability of the loosely-coupled algorithm are investigated for the following two cases of different strength
5.2. Numerical Examples

in the thermal interaction:

**Case-a**

\[
\begin{align*}
  k_1 &= 1600, \quad \rho_1 = 7500, \quad c_{p,1} = 0.5, \\
  k_2 &= 1, \quad \rho_2 = 1, \quad c_{p,2} = 1, \quad \nu_2 = 0.7, \quad \beta = 0.01, \quad g = 0.7 \cdot 10^7, \\
  L &= 1, \quad h = 0.2, \quad T_{ref} = 1, \quad T_H = 2, \quad T_C = 1, \\
  \frac{k_1}{k_2} &= 1600, \quad \frac{\alpha_1}{\alpha_2} = 0.4, \quad Pr = 0.7, \quad Ra = 1 \cdot 10^5,
\end{align*}
\]  

**Case-b**

\[
\begin{align*}
  k_1 &= 80, \quad \rho_1 = 7.5, \quad c_{p,1} = 0.12, \\
  k_2 &= 1, \quad \rho_2 = 1, \quad c_{p,2} = 1, \quad \nu_2 = 7, \quad \beta = 0.01, \quad g = 4.9 \cdot 10^7, \\
  L &= 1, \quad h = 0.2, \quad T_{ref} = 1, \quad T_H = 2, \quad T_C = 1, \\
  \frac{k_1}{k_2} &= 80, \quad \frac{\alpha_1}{\alpha_2} = 88.9, \quad Pr = 7, \quad Ra = 7 \cdot 10^4.
\end{align*}
\]

The ratio between the material properties of the coupled domains in (5.15) and (5.16) correspond to those of steel-air and steel-water couplings respectively. Thermal interaction is weak \((\sigma = 4.1 \cdot 10^{-4} \ll 1)\) for **Case-a**, and relatively strong for **Case-b** \((\sigma = 0.1)\).

Based on the prescribed values of the material properties (in both **Case-a** and **Case-b**), for stability \(\Omega_2\) takes the Dirichlet condition at the interface, while \(\Omega_1\) the Neumann condition.

5.2.2 Solution procedure

The solid domain \(\Omega_1\) is discretized using the finite volume method with the temperature stored in the cell center. The fluid domain \(\Omega_2\) is also discretized using the finite volume method with staggered arrangement of the variables [44]. In each of the subdomains, a uniform grid-spacing is used in both directions: for the solid domain: \(N_{1,x} = 80, N_{1,y} = 20\) with \(N\) number of cells, and for the fluid domain \(N_{2,x} = 80, N_{2,y} = 80\). Linear extrapolation from the cells in \(\Omega_1\) close to the interface, (3.7), is used to approximate the interface temperature. In both the momentum and energy equations, the second order centered scheme is used for discretizing the convective terms and the second order central differencing scheme is used to discretize the diffusive terms. In the flow solver, at each (implicit) stage, Picard iterations are used for solving the non-linear coupled equations [44]. The flow solver is iterated to a strict tolerance \((\epsilon_{iter} < 10^{-9}, \epsilon_{iter}: \text{maximum of the residuals of the momentum and energy equations})\) to eliminate iteration error as a contaminating variable in the
study; the residual $R_w^\phi$ at each iteration $w$ (of the flow solver) is computed using,

$$R_w^\phi = -\frac{\phi^w - \phi^n}{\Delta t a_{k,k}} + F_w^\phi + \frac{1}{a_{k,k}} \sum_{i=1}^{k-1} a_{ki} F_i^\phi,$$

(5.17)

where $\phi$ denotes the velocity and temperature fields. Furthermore, the linear systems in the flow and solid solvers are solved to machine precision.

For both cases $a$ and $b$, computations were carried out to steady-state from an initial state of unit temperature imposed on the global domain ($T(\mathbf{x}, t = 0) = 1$ for $\mathbf{x} \in \Omega = \Omega_1 \cup \Omega_2$). The purpose was to obtain information regarding the time-history of the solution during the transient phase. The time-history of the temperature at the interface and cavity centers, and $x$-component of the velocity at the cavity center are shown in Fig. 5.1. The solution reaches steady-state at $t \approx 0.3$ for Case-$a$ and $t \approx 0.2$ for Case-$b$. The monolithic approach of Schäfer and Teschauer [38] is used for the computations (a single temperature equation is solved across both the subdomains while using a separate flow field solver in the fluid subdomain). The fourth order ESDIRK (ESDIRK4) with time step-size of $\Delta t = 5 \times 10^{-4}$ was used for time integration.

![Figure 5.1: Time-history of (a) the temperature at the interface and cavity centers and (b) $x$-component of the velocity at the center of the square enclosure.](image)

5.2.3 Temporal accuracy

In order to perform the accuracy analysis, computations are first performed with the monolithic solver to time level $t_{IC}$ from an initial state of unit temperature imposed on global domain. This is done to step over the time that is required for the heat (thermal penetration depth) to travel from the bottom boundary to the interface (thermal interaction between the two subdomains has been initiated at
5.2. Numerical Examples

The fifth order ESDIRK (ESDIRK5) with time step-size of $\Delta t_{IC}$ is used for time integration. For Case-a, $t_{IC} = 0.01$ and $\Delta t_{IC} = 1 \cdot 10^{-4}$, and for Case-b, $t_{IC} = 1 \cdot 10^{-4}$ and $\Delta t_{IC} = 2 \cdot 10^{-5}$. The obtained solution at $t_{IC}$ is used as initial condition for the problem.

The coupled problem is advanced in time to $t_{final}$ with the loosely-coupled algorithm and by using various time integration schemes (for Case-a, $t_{final} = 0.06$, and for Case-b, $t_{final} = 0.02$). As Fig. 5.1 demonstrates, the solution at $t_{final} + t_{IC}$ is within the transient phase. For each case, the partitioned solution at $t_{final}$ was compared to that of the temporally exact solution (defined as the monolithic solution at $t_{final}$ obtained using a fine time step: ESDIRK5 is used for time integration with $\Delta t_{fine} = 5 \cdot 10^{-4}$ for Case-a, and $\Delta t_{fine} = 2 \cdot 10^{-5}$ for Case-b). To investigate how well the coupled problem is solved compared to the monolithic approach, computations are also carried out with the monolithic solver.

The time integration error ($\epsilon_t$) is defined as the difference between the temporally exact solution and the monolithic solution at $t_{final}$ obtained with a certain time step which is coarser relative to $\Delta t_{fine}$. The difference between the temporally exact solution and the partitioned solution at $t_{final}$ is defined as the total error in the partitioned solution ($\epsilon_{total}$) and represents the sum of the time integration error ($\epsilon_t$) and partitioning error ($\epsilon$), $\epsilon_{total} = \epsilon_t + \epsilon$. For $\epsilon_{total}$ to be of the same order as $\epsilon_t$, the partitioning error $\epsilon$ needs to be at least of the same order as $\epsilon_t$. In Fig. 5.2, for both Case-a and Case-b, the total error in the global temperature field obtained with the loosely-coupled algorithm (integrating $\Omega_1$ first, BGS-12) is shown as a function of time step size. Also shown, is the corresponding (time integration) error in temperature field obtained using the monolithic approach.

The design orders of the IMEX schemes are clearly observable for Case-a, as the results in Fig. 5.2a demonstrate. Therefore, there is no need to perform additional interface iterations at each stage to retrieve the time integration’s design order. In retaining the design order, as Fig. 5.3a and Fig. 5.3b demonstrate, the updated interface conditions must be used in evaluating the stage residual functions, $F_m^{(k)}$, otherwise order reduction occurs (in the figures, compare third and fourth order IMEX(3-4),BGS-12 with IMEX(3-4)-OR,BGS-12).

For a time-accurate partitioned solution, the partitioning error ($\epsilon$) should be as low as possible, desirably below the time integration error such that the partitioning error is not the dominant source of error in the partitioned solution (hence $\epsilon_{total} \approx \epsilon_t$). Otherwise the temporal accuracy of the partitioned solution is reduced. Below we investigate the possible influence that the order with which the domains are integrated, and the strength of the thermal interaction may have on accuracy.

In Fig. 5.3, by comparing the total error in the temperature field obtained with the two different integration sequences with the corresponding (time integration) error in the monolithic solution, it is observed that the partitioned solution obtained by integrating $\Omega_1$ first (BGS-12) is more accurate than that of BGS-21 and for this test-case is as accurate as the monolithic solution. In solving the coupled problem
Figure 5.2: Total error in the global temperature field ($\varepsilon_{T,\text{total}}$) as a function of $\Delta t$ for (a) Case-a, (b) Case-b. In the figures, CN refers to monolithic solution obtained with Crank-Nicolson, ESDIRK 3 – 5 refer to the monolithic solutions obtained using the 3rd-5th order ESDIRK schemes. The solution obtained using the predictor-corrector Crank-Nicolson scheme of [22] is denoted by pred-corr CN, and the solutions obtained using the 3rd-5th order IMEX schemes are denoted by IMEX 3 – 5.

Figure 5.3: The total error in the global temperature field as a function of time-step size for Case-a. In the figures, the partitioned solutions obtained by integrating $\Omega_1$ first are indicated by BGS-12, while those obtained by integrating $\Omega_2$ first are indicated by BGS-21. IMEX(3-4)-OR,BGS-12 refer to the partitioned solutions obtained using IMEX(3-4) for time integration where the updated interface conditions are not used in the evaluation of the stage residual functions, and hence order reduction occurs.

using BGS-21, the partitioning error (as a result of segregated solve of the interface equations) is placed entirely in the continuity of the interface temperature equation.
and therefore this equation is solved approximately while the continuity of the interface heat flux is satisfied exactly. This is in opposite to solving the problem using BGS-12. In general it is not clear which approximation (having a discontinuity in the interface heat flux or interface temperature) is less disadvantageous and seems to be an issue which is problem dependent. At least for this test case, as the results in Fig. 5.3 demonstrate, using BGS-12 provides a solution which is more accurate than BGS-21.

Furthermore, the temporal convergence character of the total error of the solution using BGS-21 is also influenced by the partitioning error; to observe the full-design orders smaller time-step sizes need to be considered. It is noted that by solving the test-case on coarser grids of the fluid and solid subdomains (hence smaller Fourier numbers $\Delta x_m^2$ relative to the current mesh) full-design orders has been observed.

By comparing the results of cases a and b in Fig. 5.2a and Fig. 5.2b, it can be inferred that as the strength of the thermal interaction increases ($\sigma \rightarrow 1$), so does the partitioning error. As a result, the accuracy of the partitioned solution deteriorates (this holds irrespective of the sequence with which domains are integrated). Furthermore, it is observed that as the order of the time integration scheme increases, the partitioning error increases. It is noted that similar to results of Case-a obtained using BGS-21, to observe the full-design orders smaller time-step sizes need to be considered.

### 5.2.4 Stability

By neglecting flow in the fluid domain $\Omega_2$, and noting that the left and right boundaries of the problem are insulated (Fig. 4.2), the coupled problem reduces to the 1-D model problem of section 2.2 where the governing equation within each subdomain is conduction. Following the discussion in section 5.1.1, first the stability of the IMEX schemes is investigated numerically for the 1-D model problem. We investigate whether similar to the stability of Crank-Nicolson (5.14), a relation between $\sigma$ and stability of the IMEX schemes can be observed; of particular interest is a condition which will indicate the possibility of using large Fourier number of subdomains. The results of the 1-D model problem will also serve as reference for the 2-D CHT test-case.

#### 5.2.4.1 Stability of the 1-D model problem

For the analysis, three different values of $\sigma$ are considered: $4.1 \times 10^{-4}$ (Case-a), 0.1 (Case-b), and 1. For case of $\sigma = 1$, material properties of both subdomains are set to 1. A step initial condition is imposed on the global domain: $T(y, t = 0) = 2, y \in \Omega_1$ and $T(y, t = 0) = 1, y \in \Omega_2$. The non-interface boundary conditions are kept unchanged and set to $T_1(y = -h, t) = 2$ and $T_2(y = L, t) = 1$. To minimize the influence of the non-interface boundary conditions on the analysis, the length of the subdomains in the $y$-direction (in Fig. 4.2) are extended to sufficiently large values;
Table 5.1: *Approximate* $\Delta t$ and corresponding Fourier numbers $d_m$ at which simulations become unstable for (a) Case-a, (b) Case-b, and (c) Case $\sigma = 1$.

<table>
<thead>
<tr>
<th></th>
<th>$\Delta t$</th>
<th>$d_1$</th>
<th>$d_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a) $\sigma = 4.1 \times 10^{-4}$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pred-Corr CN</td>
<td>$3.2 \cdot 10^{-1}$</td>
<td>$1.4 \cdot 10^3$</td>
<td>$2.0 \cdot 10^3$</td>
</tr>
<tr>
<td>IMEX-3</td>
<td>$5.9 \cdot 10^2$</td>
<td>$2.5 \cdot 10^6$</td>
<td>$3.8 \cdot 10^6$</td>
</tr>
<tr>
<td>IMEX-4</td>
<td>$1.4 \cdot 10^3$</td>
<td>$6.0 \cdot 10^6$</td>
<td>$9.0 \cdot 10^6$</td>
</tr>
<tr>
<td>IMEX-5</td>
<td>$1.3 \cdot 10^2$</td>
<td>$5.5 \cdot 10^5$</td>
<td>$8.3 \cdot 10^5$</td>
</tr>
<tr>
<td>(b) $\sigma = 1 \times 10^{-1}$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pred-Corr CN</td>
<td>$7.5 \cdot 10^{-5}$</td>
<td>$6.7 \cdot 10^1$</td>
<td>$4.8 \cdot 10^{-1}$</td>
</tr>
<tr>
<td>IMEX-3</td>
<td>$6.7 \cdot 10^{-4}$</td>
<td>$6.0 \cdot 10^2$</td>
<td>$4.3 \cdot 10^0$</td>
</tr>
<tr>
<td>IMEX-4</td>
<td>$2.8 \cdot 10^{-3}$</td>
<td>$2.5 \cdot 10^3$</td>
<td>$1.8 \cdot 10^1$</td>
</tr>
<tr>
<td>IMEX-5</td>
<td>$3.1 \cdot 10^{-4}$</td>
<td>$2.7 \cdot 10^2$</td>
<td>$1.9 \cdot 10^0$</td>
</tr>
<tr>
<td>(c) $\sigma = 1$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pred-Corr CN</td>
<td>$8.34 \cdot 10^{-5}$</td>
<td>$8.3 \cdot 10^{-1}$</td>
<td>$5.3 \cdot 10^{-1}$</td>
</tr>
<tr>
<td>IMEX-3</td>
<td>$3.2 \cdot 10^{-4}$</td>
<td>$3.2 \cdot 10^0$</td>
<td>$2.0 \cdot 10^0$</td>
</tr>
<tr>
<td>IMEX-4</td>
<td>$1.8 \cdot 10^{-4}$</td>
<td>$1.8 \cdot 10^0$</td>
<td>$1.2 \cdot 10^0$</td>
</tr>
<tr>
<td>IMEX-5</td>
<td>$2.1 \cdot 10^{-4}$</td>
<td>$2.1 \cdot 10^0$</td>
<td>$1.3 \cdot 10^0$</td>
</tr>
</tbody>
</table>

the thermal penetration depth $\delta_m \sim \sqrt{\alpha_m t}$ within each subdomain at the time at which instability occurs is far away from the boundaries. The number of cells in both domains were accordingly increased to keep the grid size in the $y$-direction unchanged compared to the CHT case.

For each case, $\Delta t$ is incremented until the computations become unstable. The *approximate* $\Delta t$ and the corresponding Fourier numbers of the subdomains at which simulations become unstable are presented in Table 5.1(a)–(c). Computations using both the integration sequences (BGS-12,BGS-21) provided similar results.

For the predictor-corrector Crank-Nicolson scheme, substituting the model parameters of Case-a and Case-b, and case of $\sigma = 1$ into (5.13) (with $\gamma = \frac{2}{3}$), the expected $\Delta t$ values at which instabilities initiate are respectively $\Delta t = 0.31$, $\Delta t = 7.4 \cdot 10^{-5}$, and $8.33 \cdot 10^{-5}$. As the results in Table 5.1(a)–(c) show, for the three cases instability initiates when the criterion (5.13) is not satisfied. This also verifies the numerical procedure used to investigate the stability of the algorithm.

For the high order IMEX schemes, as the results in Table 5.1(a)–(c) demonstrate, the loosely-coupled algorithm becomes unstable for sufficiently large values of the Fourier numbers of the coupled domains. A similar observation is made for the predictor-corrector Crank-Nicolson. In addition, the IMEX schemes demonstrate better stability properties compared to the Crank-Nicolson scheme for all the con-
5.2. Numerical Examples

Table 5.2: Influence of grid spacing on stability.

<table>
<thead>
<tr>
<th>σ</th>
<th>$\Delta t_{ref}$</th>
<th>$(d_1 d_2)_{ref}$</th>
<th>$\Delta y_{1,F} = 2\Delta y_1$</th>
<th>$\Delta y_{2,F} = 2\Delta y_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.8 $\cdot 10^{-4}$</td>
<td>1.4 $\times 10^3$</td>
<td>5.3 $\times 10^{13}$</td>
<td>2.1</td>
<td>1.1</td>
</tr>
<tr>
<td>1.3 $\cdot 10^{-1}$</td>
<td>2.8 $\times 10^{-3}$</td>
<td>4.5 $\times 10^{4}$</td>
<td>2.4</td>
<td>1.4</td>
</tr>
<tr>
<td>1 $\cdot 10^0$</td>
<td>1.8 $\times 10^{-4}$</td>
<td>2.1 $\times 10^0$</td>
<td>2</td>
<td>1</td>
</tr>
</tbody>
</table>

considered σ values; while they outperform Crank-Nicolson for case of σ ≪ 1, they are marginally better for σ = 1.

For Crank-Nicolson, the results in the tables can be explained using the available stability criterion ($\sigma \sqrt{d_1 d_2} < \frac{2}{3}$). When σ ≪ 1, it follows that $\sqrt{d_1 d_2}$ can take large values ($\sqrt{d_1 d_2} \gg 1$) while still adhering to the criterion and vice-versa. Analyzing the results in the tables, suggest a similar trend for the IMEX schemes. Comparing the stability results of Case-a with the corresponding ones for Case-b and case of σ = 1, demonstrates that when the thermal interaction between the subdomains is weak (σ ≪ 1), the product $\sqrt{d_1 d_2}$ is large and the IMEX schemes remain stable to large Fourier numbers. However, as σ → 1 (Case-b, σ = 1), $\sqrt{d_1 d_2}$ reduces significantly, and the Fourier numbers of the domains are small. Hence, the results imply that the product $\sigma \sqrt{d_1 d_2}$, which in (B.2) was shown to be part of the coupling term in the discretization of the interface node, has an influential effect on the stability of the IMEX schemes. More importantly, σ can be identified as the single parameter which provides the condition (σ ≪ 1) for using large Fourier numbers (the reason for using implicit time integration).

In the stability criterion (5.13) for the Crank-Nicolson scheme, the Δt for stability depends linearly on the mesh spacings Δy_m. Alternatively, from (5.14), it is observed that a change in the mesh spacing results in a change in Δt such that the product of the Fourier numbers of the subdomains remains constant, i.e. $d_1 d_2 < \left(\frac{2}{\sigma}\right)^2$. A stability investigation was performed using IMEX4, to see whether similar observations can be made for the high order IMEX schemes; the grid in one domain is increased by a factor of two while retaining the grid size fixed in the other. As the results in Table 5.2 show, by increasing the mesh spacing by a factor of two, the approximate Δt at which instability initiates (denoted in the table by $\Delta t_{ref}$) reduces by approximately the same factor relative to $\Delta t_{ref}$. Furthermore, the product of the Fourier numbers of the coupled domains is approximately the same as the reference $(d_1 d_2)_{ref}$.

The stability results in Table 5.1 and Table 5.2 were obtained assuming semi-infinite subdomains. Computations were also carried out for cases a and b to investigate the extend to which the stability results of the IMEX schemes may be influenced by the non-interface boundary conditions placed at a finite distance from the interface (at y = L and y = −h) in Fig. 4.2).
Table 5.3: Approximate $\Delta t$ and the corresponding Fourier numbers of the subdomains at which simulations become unstable for Case-b and finite length of subdomains.

<table>
<thead>
<tr>
<th>$\sigma = 1 \times 10^{-1}$</th>
<th>$\Delta t$</th>
<th>$d_1$</th>
<th>$d_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>IMEX-3</td>
<td>$7.1 \cdot 10^{-4}$</td>
<td>$6.4 \cdot 10^2$</td>
<td>$4.5 \cdot 10^0$</td>
</tr>
<tr>
<td>IMEX-4</td>
<td>$2.6 \cdot 10^{-3}$</td>
<td>$2.3 \cdot 10^3$</td>
<td>$1.7 \cdot 10^1$</td>
</tr>
<tr>
<td>IMEX-5</td>
<td>$3.1 \cdot 10^{-4}$</td>
<td>$2.8 \cdot 10^2$</td>
<td>$2.0 \cdot 10^0$</td>
</tr>
</tbody>
</table>

The same length and number of cells in the $y$-direction of the CHT problem were used for this 1-D test case. For Case-b, the results are shown in Table 5.3. A maximum difference of 6% with the results of the semi-infinite subdomains in Table 5.1(b) is observed. The difference was found to be larger for Case-a; as an example, for IMEX-4 instability initiates at a $\Delta t$ approximately 3 times larger than the corresponding result in Table 5.1(a).

The governing non-dimensional parameters of the 1-D model problem, due to lack of convection, are $\frac{\alpha_1}{\alpha_2}$ and $\frac{k_1}{k_2}$. While the stability of the high order IMEX schemes is influenced by the two ratios, however, for the purpose of our analysis, it is more appropriate to use $\sigma = \left(\frac{k_1}{k_2}\sqrt{\frac{\alpha_1}{\alpha_2}}\right)$. For a given strength of thermal interaction, we are interested in whether it is possible to take large Fourier numbers as desired using the loosely coupled IMEX schemes. $\sigma$ (an indicator of the strength of the coupling), as demonstrated in this section, does serve the purpose and provides an estimate of cases ($\sigma \ll 1$) where the high order IMEX schemes should be applied to.

5.2.4.2 Stability of the CHT problem

Returning to the CHT test-case, the problem is two dimensional. Furthermore, the fluid domain includes more complex physics, i.e. coupled-nonlinear equations. While the governing non-dimensional parameters of 1-D model problem are $\frac{\alpha_1}{\alpha_2}$ and $\frac{k_1}{k_2}$, the CHT test-case includes $Pr$ and $Ra$ as two additional parameters. Hence, for 2-D (and 3-D) computations, satisfying the stability criteria for the 1-D model problem is necessary, but may not be a sufficient one [11]. Therefore, stability of the coupling algorithm in solving the CHT problem was also investigated numerically, in a similar manner as the 1-D problem.

For Case-a, numerical computations using the high order IMEX schemes with $\Delta t$ values sufficient to capture the transients were performed without encountering stability issues (maximum considered $\Delta t$ was $1 \cdot 10^{-2}$). For Case-b, a noticeable difference with the stability results of the 1-D model problem in Table 5.3 was not observed. Similar observations were made when the $Pr$ and $Ra$ numbers were separately reduced by a factor of 10 while all the other parameters were fixed. Therefore, at least for this particular test-case, the results of the CHT computations suggest a marginal influence of $Pr$, $Ra$, and other possible contributing factors such as two dimensionality on stability.
5.2.4.3 Intermediate conclusions

The main conclusion which should be drawn from the stability investigation on the simplified 1-D and the 2-D CHT test-cases is the possibility to use the single variable $\sigma$, to identify a class of problems which the loosely coupled IMEX schemes are appropriate to apply to. This is a particularly useful result, given the absence of an analytical stability criterion. Based on the analysis, it may be concluded that when the thermal interaction between the subdomains is weak ($\sigma \ll 1$), the IMEX schemes remain stable to large Fourier numbers $d_m$. However, as $\sigma$ approaches unity, the stability and accuracy of the schemes reduce.

The possibility to use large Fourier numbers for weakly-coupled problems, is an indication that time-step size is restricted by accuracy rather than stability, at least on reasonable grids. This is demonstrated for the CHT test-case under study: since the transients to steady state for cases $a$ and $b$ are completed within $\approx t = 0.3$ (see Fig. 5.1), taking time-step sizes in the order of $\Delta t = 10^{-1}$ can be considered large and correspond to a time which most of the transients have passed. For Case-a ($\sigma \ll 1$), computations with the largest considered time-step size $\Delta t = 1 \cdot 10^{-2}$ sufficient to capture the transients were stable. However, for case-b ($\sigma = 0.1$), the time-step sizes at which instability occur, Table 5.3, are adequate to capture the transient phase.

5.2.5 Computational efficiency assessment

While in the loosely coupled multi-stage IMEX schemes a single interface iteration is performed at each (implicit) stage, in the predictor-corrector Crank-Nicolson scheme, only one is performed per time-step. However, for the same time-step, the high order IMEX schemes generally provide temporally more accurate solutions. For the CHT test-case considered here, we investigate whether the additional work per time step of the IMEX schemes is compensated by the gain in accuracy compared to Crank-Nicolson and BDF2 schemes. Based on the results of the accuracy and stability investigation for the IMEX schemes discussed above, only Case-a where the thermal interaction between the two domains is weak ($\sigma \ll 1$) is considered.

Prior to discussing the results, as an illustration of the quality of the solution at different error levels, the variation with time of the temperature and $x$-component of the velocity at the center of the cavity is demonstrated in Fig. 5.4. The partitioned solutions are obtained using the predictor-corrector Crank-Nicolson and as reference, the data from the temporally exact solution are also included. To capture the transients with reasonable accuracy using the Crank-Nicolson scheme, a time-step size in the range of $1 \cdot 10^{-3} \leq \Delta t \leq 2 \cdot 10^{-3}$ should be considered (as Fig. 5.4b shows).

The total error in the temperature field and $x$-component of the velocity field are plotted against the work in respectively Fig. 5.5a and Fig. 5.5b for several time integration schemes. The work is defined as the total number of implicit calculations.
during the simulation \( W = (s - 1) \frac{t_{\text{final}}}{\Delta t} \), with \( s - 1 \) being the number of implicit stages per time-step). The temporal accuracies of the velocity and temperature fields using a time-step size in the range of \( 1 \cdot 10^{-3} \leq \Delta t \leq 2 \cdot 10^{-3} \) are approximately in the range of \( 1 \cdot 10^{-3} \leq \varepsilon_u^{\text{total}} \leq 1 \cdot 10^{-2} \) and \( 1 \cdot 10^{-4} \leq \varepsilon_T^{\text{total}} \leq 1 \cdot 10^{-3.5} \) respectively. Comparing Fig. 5.4a and Fig. 5.4b, shows that for a given time step size, the error in capturing the transients of the solution is higher in the velocity field. Hence, we continue the discussion only considering results in Fig. 5.5b.

Figure 5.4: Time-history of (a) the temperature and (b) x-component of the velocity at the center of the square enclosure. The results are obtained using the predictor-corrector Crank-Nicolson scheme. As reference, the results of the temporally exact solution obtained with ESDIRK-5 are also included.

Figure 5.5: Work-Accuracy character of several time integration schemes for obtaining the solution to: (a) the temperature field, (b) x-component of the velocity.
As Fig. 5.5b demonstrates, for reasonable accuracies of $1 \cdot 10^{-3} \leq \epsilon^u_{\text{total}} \leq 1 \cdot 10^{-2}$, both IMEX4 and IMEX5 reduce the computational work relative to BDF2 by approximately a factor of $1.9 - 2.7$. IMEX-4 and IMEX-5 are as efficient as Crank-Nicolson for $\epsilon^u_{\text{total}} \approx 10^{-2}$ and for an accuracy of $\epsilon^u_{\text{total}} \approx 10^{-3}$ are more efficient than Crank-Nicolson by a factor of 1.5. As the figure demonstrates, for high-accuracy solutions, $\epsilon^u_{\text{total}} < 10^{-4}$, all the three IMEX schemes are computationally more efficient than both BDF2 and Crank-Nicolson.

The A-stable Crank-Nicolson scheme performs well compared to the L-stable time-integration schemes, in particular BDF2. Decline in the efficiency of the Crank-Nicolson may be expected when the solution varies rapidly with time.

5.2.6 Case of temperature dependent thermal conductivity

Now the complexity of the coupled problem is increased by assuming that conductivities of the two subdomains vary with temperature according to the function:

$$k_m(T_m) = k_{m,0}(1 + \lambda_{m,1}(T_m - T_{\text{ref}})^{\gamma_{m,1}} + \lambda_{m,2}(T_m - T_{\text{ref}})^{\gamma_{m,2}}),$$

(5.18)

where $k_{m,0}$ is the conductivity at the initial state ($t = 0$), and $\lambda_{m,1}$, $\lambda_{m,2}$, $\gamma_{m,1}$, and $\gamma_{m,2}$ are constants. We wish to examine the order-preservation of the loosely-coupled solution algorithm under the condition of nonlinear coupling terms.

The value of the thermal conductivity at a control volume (or cell) face is evaluated by using the harmonic averaging of the cell-center conductivities (obtained with (5.18)) adjacent to the face $k_{\text{face}} = \frac{2k_{i}k_{i+1}}{k_{i} + k_{i+1}}$ [27]. For the faces located at the boundaries of the subdomains at which the temperature condition is imposed, the conductivity is obtained by using (5.18).

When the domain which requires the flux condition at the interface is integrated first, BGS-12, the loosely-coupled algorithm presented in section 5.1 can be used without any further considerations in addition to taking into account that $k_{2,2} = k_{2,2}(T_{2,2})$. However, when the domain which requires the temperature at the interface is integrated first, a few issues need to be discussed. In solving for $T^{(k)}_2$, the flux predictor (5.2) and state (temperature) predictor (5.5) no longer lead to the same prediction of $f_{21}^*$ in (5.3) due to the nonlinearity of the the interface heat conductivity ($k_{2,2} = k_{2,2}(T_{2,2})$). As pointed out in section 5.1, for (5.3) to be equivalent to (5.1) where the coupling term is integrated using an Explicit RK, the following prediction of $f_{21}^{(s)}$ needs to be considered (flux predictor):

$$f_{21}^{(s)} = \sum_{i=1}^{k-1} \frac{a_{ki}^E - a_{ki}^I}{a_{kk}^I} f_{21}^{(i)} = \frac{1}{\Delta x_{2,2}h} \sum_{i=1}^{k-1} \frac{a_{ki}^E - a_{ki}^I}{a_{kk}^I} k_{2,2}(T_{2,2}^{(i)}) T_{2,2}^{(i)}.$$

(5.19)

Furthermore, in solving for $T^{(k)}_2$, an approximation to the interface conductivity, $k_{2,2}$, which appears in the coefficient matrix $A_2$ (as a result of spatial discretization
of the cells next to the interface (3.6) needs to be considered. One option is to make use of the available interface conductivities evaluated at the previous stages. Here, an expression similar to state predictor given by (5.5) is considered for computing $k_{2,I}^{(s)}$:

$$k_{2,I}^{(s)} = \sum_{i=1}^{k-1} \frac{a_k^E - a_k^I}{a_{kk}} k_{2,I}(T_{2,I}^{(i)}) .$$

(5.20)

After the computation of $T_{2,I}^{(k)}$, the interface flux is evaluated using:

$$q_{1,I}^{(s)} = q_{2,I}^{(s)} = -\left( \frac{k_{2,I}^{(s)}}{\Delta x_{2,b}} T_{2,1}^{(k)} - f_{21}^{(s)} \right)$$

$$= -\sum_{i=1}^{k-1} \frac{a_k^E - a_k^I}{a_{kk}} k_{2,I}^{(s)} \frac{k_{I}}{\Delta x_{2,b}} (T_{2,1}^{(k)} - T_{2,I}^{(i)}),$$

(5.21) (5.22)

where, $k_{2,I}^{(s)} = k_{2,I}(T_{2,I}^{(s)})$. The rest of the algorithm remains unchanged.

An alternative but not equivalent approach is to use the state predictor in the evaluation of $f_{21}^{(s)}$. By expressing $f_{21}^{(s)}$ as $f_{21}^{(s)} = \frac{k_{2,I}^{(s)}}{\Delta x_{2,b}} T_{2,I}^{(s)}$, it is observed that approximations to $k_{2,I}^{(s)}$ and $T_{2,I}^{(s)}$ are required. In this approach, first $T_{2,I}^{(s)}$ is evaluated using the state predictor (5.5). $k_{2,I}^{(s)}$ is then computed by substituting the obtained value for the interface temperature into corresponding conductivity function ($k_{2,I}^{(s)} = k_{2,I}(T_{2,I}^{(s)})$). The computed value of $k_{2,I}^{(s)}$ is used both in the coupling term and in the appropriate term in the coefficient matrix $A_2$. After solving for $T_{2,I}^{(k)}$, the interface flux is evaluated using $q_{1,I}^{(s)} = q_{2,I}^{(s)} = -\frac{k_{2,I}^{(s)}}{\Delta x_{2,b}} (T_{2,1}^{(k)} - T_{2,I}^{(s)})$ where $k_{2,I}^{(s)}$ and $T_{2,I}^{(s)}$ are known.

The model parameters of Case-a along with the following values of the parameters in (5.18) are used in this test case (the conductivities are weak functions of temperature):

$$k_{1,0} = 1600, \quad \lambda_{1,1} = -0.0062, \quad \lambda_{1,2} = 0, \quad \gamma_{1,1} = 1.5, \quad \gamma_{1,2} = 0, \quad T_{ref} = 1$$

(5.23)

$$k_{2,0} = 1, \quad \lambda_{2,1} = 0.64, \quad \lambda_{2,2} = -0.085, \quad \gamma_{2,1} = 1.0, \quad \gamma_{2,2} = 1.5.$$

The CHT test-case is solved using the loosely-coupled algorithm noting the modifications discussed above. Both the flow and solid solvers are iterated to a specified tolerance ($10^{-9}$) to resolve the non-linearities present within each subdomain. The convergence of the total error in the global temperature field using the loosely-coupled algorithm with time-step size is investigated in the same manner discussed earlier. The results are shown in Fig. 5.6. The design order of IMEX-3 is clearly observable for BGS-12. Similar to the case of linear conductivities considered earlier, the accuracy of the solution using BGS-21 is deteriorated due to the partitioning
error (and smaller time-steps need to be considered to observe the full design order). As a result of the non-linear coupling terms, the two integration sequences may also exhibit different stability behaviors, as demonstrated in [22] for the Crank-Nicolson scheme.

In solving the coupled problem using BGS-21, the approach which makes use of the state predictor, is not equivalent to integrating the complete coupling term using an ERK and therefore, there is the possibility of order reduction. However, as the results in the figure demonstrate, at least for this test case order reduction is not observed (IMEX3, BGS-21, State Pred). Furthermore, the partitioned solutions obtained with both the alternatives (flux and state predictors), are approximately of equal accuracy relative to the monolithic solution.

![Graph showing total error vs. time-step](image)

**Figure 5.6:** Total error in the global temperature field as a function of $\Delta t$ for case with nonlinear conductivity of subdomains.

### 5.3 Conclusions

In order to reduce the computational expense of solving time-accurate unsteady CHT problems using a loosely-coupled partitioned approach, we considered the use of high order implicit time integration schemes which have the potential to improve the computational efficiency relative to the commonly used second order implicit schemes. In particular, we presented a loosely-coupled solution algorithm where high order implicit-explicit (IMEX) Runge-Kutta schemes are employed for time integration. The high order IMEX schemes consist of the explicit first-stage singly diagonally implicit Runge-Kutta (ESDIRK) schemes, for advancing the solution in time within each separate fluid and solid subdomain, and the explicit Runge-Kutta (ERK) schemes, for explicit integration of part of the coupling terms.

To demonstrate the applicability and the temporal order preservation (without subiterating) of this loosely-coupled algorithm, an unsteady conjugate natural
convection in an enclosure was considered as a numerical example. Furthermore, the stability of the algorithm was investigated numerically and compared with the results of the analytical stability analysis for the Crank-Nicolson scheme. The analysis demonstrated that the loosely-coupled IMEX algorithm becomes unstable for sufficiently large Fourier numbers. Furthermore, when the ratio of the thermal effusivities of fluid and solid subdomains is much smaller than unity, it is possible to use large Fourier numbers, indicating that time-step size is restricted by accuracy rather than stability. In addition, the results showed better stability properties of the IMEX schemes compared to the Crank-Nicolson scheme.

Furthermore, the (computational) work-(temporal) precision character of the high order IMEX and the commonly used second order implicit schemes in solving the CHT test-case was compared over a range of accuracy requirements; for time-accurate solutions, the fourth and fifth order IMEX schemes are 1.5 times more efficient than the Crank-Nicolson scheme and 2.7 times more efficient than the second order backward difference (BDF2) scheme. The computational gain is higher for smaller tolerances.
Chapter 6

High order ESDIRK schemes and a strongly-coupled solution algorithm


In the previous chapter, it was observed that when the thermal interaction between the domains became stronger, the stability and the temporal accuracy of the loosely-coupled IMEX algorithm reduced. For such cases, it is more appropriate to use a strongly-coupled solution algorithm.

In this chapter a time-accurate strongly-coupled solution algorithm is considered where the high order ESDIRK schemes are used for time integration within each separate fluid and solid subdomains. Interface iterations (subiterations) are performed (at each stage) to retain the stability and/or to increase the accuracy of the partitioned solution. Dirichlet-Neumann interface conditions are used for the spatial coupling of the subdomains at the interface. Stability and rate of convergence of performing (Gauss-Seidel) subiterations at each stage of the ESDIRK schemes are analyzed analytically. Numerical examples are considered in order to validate the performed analytical stability analysis.

Furthermore, by considering a strongly coupled CHT test-case, the computational efficiency of the algorithm relative to the strongly-coupled Crank-Nicolson and the high order loosely-coupled IMEX algorithm is assessed.
6.1 Stability analysis

In this section we study the stability and rate of convergence of (Gauss-Seidel) interface iterations at each stage of the ESDIRK schemes in a strongly-coupled solution algorithm. Dirichlet-Neumann interface conditions are used for spatial coupling between the subdomains where, at the interface, the Dirichlet condition is applied to one subdomain and the Neumann condition to the other subdomain. The analysis follows that of Henshaw and Chand [14] where the \( \theta \) scheme was used for time integration.

The model problem which is used to analyze the stability of the partitioned algorithm, consists of two thermally coupled rectangular domains \( \Omega_1 = [-L_1,0] \times [0,2\pi] \) and \( \Omega_2 = [0,L_2] \times [0,2\pi] \) with their common interface at \( \partial \Omega_I = 0 \times [0,2\pi] \). The governing equation within each subdomain is transient conduction. The following set of coupled PDEs along with their respective boundary and initial conditions is considered:

\[
\frac{\partial T_m}{\partial t} = \alpha_m \nabla^2 T_m + f_m(x,t), \quad \text{for} \ x \in \Omega_m, m = 1, 2 \quad (6.1)
\]

\[
T_2|_I = T_1|_I, \quad (6.2)
\]

\[
k_1 \frac{\partial T_1}{\partial x}|_I = k_2 \frac{\partial T_2}{\partial x}|_I, \quad (6.3)
\]

\[
T_1(-L_1,y) = g_1(y), \quad T_2(L_2,y) = g_2(y), \quad (6.4)
\]

\[
T_m(x,0) = T_m^0(x), \quad \text{for} \ x \in \Omega_m, m = 1, 2 \quad (6.5)
\]

where solutions which are \( 2\pi \)-periodic in the \( y \)-direction are sought. The problem is discretized in time but kept continuous in space. Application of the ESDIRK schemes to (6.1) yields:

\[
\vartheta_m^{(k)}(x) - \vartheta_m^n(x) = \Delta t \sum_{i=1}^{k} a_{ki} (\alpha_m \nabla^2 \vartheta_m + f_m(x,t))^{(i)} \quad \text{for} \ x \in \Omega_m, m = 1, 2 \quad (6.6)
\]

where \( \vartheta_m^{(k)}(x) \approx T_m(x,t^{(k)}) \) is the monolithic solution to the coupled problem at \( t^{(k)} = t^n + c_k \Delta t \). After some re-arrangements the above equation along with the corresponding boundary and initial conditions can be written as:

\[
\nabla^2 \vartheta_m^{(k)} - \frac{1}{\Delta t a_{kk} \alpha_m} \vartheta_m^{(k)} = F_m \quad \text{for} \ x \in \Omega_m, m = 1, 2 \quad (6.7)
\]

\[
\vartheta_2^{(k)}|_I = \vartheta_1^{(k)}|_I \quad (6.8)
\]

\[
k_1 \frac{\partial \vartheta_1^{(k)}}{\partial x}|_I = k_2 \frac{\partial \vartheta_2^{(k)}}{\partial x}|_I \quad (6.9)
\]

\[
\vartheta_1^{(k)}(-L_1,y) = g_1(y), \quad \vartheta_2^{(k)}(L_2,y) = g_2(y) \quad (6.10)
\]

\[
\vartheta_m^0(x) = T_m^0(x) \quad \text{for} \ x \in \Omega_m, m = 1, 2 \quad (6.11)
\]
where

\[
F_m = \frac{-1}{\alpha_m} f^{(k)}(x) - \frac{1}{\Delta t a_{kk} \alpha_m} \left[ \varphi_m^0(x) + \sum_{i=1}^{k-1} a_{ki} \left( \alpha_m \nabla^2 \varphi_m(x) + f(x,t) \right)(i) \right]
\]  

are the known explicit contributions. Here, Block Gauss-Seidel iterations (the coupled domains are solved in a sequential manner) are considered for solving the coupled implicit equations (6.7)-(6.10) to obtain \( \varphi_m^{(k)} \). If \( \{ \varphi_m^j \}_{j \geq 0} \) denotes a sequence of iterates, we would like to see if the sequence converges to the monolithic solution, i.e. \( \varphi_m^j \to \varphi_m^{(k)} \) as \( j \to \infty \) starting from an initial guess. Assuming that the Neumann condition is applied to \( \Omega_1 \) and the Dirichlet condition to \( \Omega_2 \), then we define the following iteration for \( j > 0 \), where \( \Omega_1 \) is solved first:

\[
\nabla^2 \varphi_m^j - \frac{1}{\Delta t a_{kk} \alpha_m} \varphi_m^j = F_m \quad \text{for} \quad x \in \Omega_m, m = 1, 2
\]  

(6.13)

\[
\varphi_m^j \big|_{\partial \Omega_m} = \varphi_m^{(k)} \big|_{\partial \Omega_m}
\]  

(6.14)

\[
k_1 \frac{\partial \varphi_m^j}{\partial x} \big|_{\partial \Omega_m} = k_2 \frac{\partial \varphi_m^{(k)} - 1}{\partial x} \big|_{\partial \Omega_m}
\]  

(6.15)

\[
\varphi_m^j (-L_1, y) = g_1(y), \quad \varphi_m^j (L_2, y) = g_2(y).
\]  

(6.16)

By subtracting a particular solution to (6.7) and (6.10) that satisfies homogeneous Dirichlet conditions at the interface, from (6.13)-(6.16), and furthermore by Fourier transforming in the \( y \) direction (with transform variable \( \kappa \)), an iteration for the partitioning error \( \hat{\epsilon}_m^j(x, \kappa) \) is obtained:

\[
\partial_x^2 \hat{\epsilon}_m^j = \beta_m \hat{\epsilon}_m^j, \quad m = 1, 2
\]  

(6.17)

\[
\hat{\epsilon}_m^j \big|_{\partial \Omega_m} = \hat{\epsilon}_m^{(k)} \big|_{\partial \Omega_m}
\]  

(6.18)

\[
k_1 \frac{\partial \hat{\epsilon}_m^j}{\partial x} \big|_{\partial \Omega_m} = k_2 \frac{\partial \hat{\epsilon}_m^{(k)} - 1}{\partial x} \big|_{\partial \Omega_m} + \psi(\kappa),
\]  

(6.19)

\[
\hat{\epsilon}_m^j (-L_1, \kappa) = 0, \quad \hat{\epsilon}_m^j (L_2, \kappa) = 0
\]  

(6.20)

where \( \beta_m \) is defined as,

\[
\beta_m = \sqrt{\kappa^2 + \frac{1}{a_{kk} \alpha_m \Delta t}}.
\]  

(6.21)

By applying the outer boundary conditions (6.20) to the general solution of (6.17) and substituting the solution into the interface boundary conditions (6.18)-(6.19), after some algebra the following equation for the amplification factor is obtained
\[ A = -\frac{k_2}{k_1} \frac{\beta_2 \tanh (\beta_1 L_1)}{\beta_1 \tanh (\beta_2 L_2)} = -\frac{k_2}{k_1} \frac{\beta_2}{\beta_1} \frac{\tanh \left( \sqrt{L_1^2 \kappa^2 + \frac{1}{a_{kk}} \left( \frac{L_1}{\delta_1(\Delta t)} \right)^2} \right)}{\tanh \left( \sqrt{L_2^2 \kappa^2 + \frac{1}{a_{kk}} \left( \frac{L_2}{\delta_2(\Delta t)} \right)^2} \right)}, \quad (6.22) \]

where \( \delta_m(\Delta t) = \sqrt{\alpha_m \Delta t} \) represents the distance that the heat diffuses in the subdomain in one time-step. Noting that time-accurate computations are being performed, it can be assumed that in many cases \( \beta_1 L_1 \gg 1 \) and \( \beta_2 L_2 \gg 1 \) for which \( \tanh (\beta_1 L_1) \approx 1 \) and \( \tanh (\beta_2 L_2) \approx 1 \). Then, for the two conditions \( \frac{1}{a_{kk}\alpha_m \Delta t} \gg \kappa^2 \) and \( \frac{1}{a_{kk}\alpha_m \Delta t} \ll \kappa^2 \), (6.22) reduces to:

\[ A \approx \begin{cases} \frac{k_2}{k_1} & \text{if } \frac{1}{a_{kk}\alpha_m \Delta t} \gg \kappa^2, \\ \frac{k_2}{k_1} \sqrt{\frac{\alpha_1}{\alpha_2}} & \text{if } \frac{1}{a_{kk}\alpha_m \Delta t} \ll \kappa^2. \end{cases} \quad (6.23) \]

Therefore, at each stage, the rate of convergence of the subiterations for smooth components of the solution (small wave numbers) is given by:

\[ |A| = \frac{k_2}{k_1} \sqrt{\frac{\alpha_1}{\alpha_2}}, \quad (6.24) \]

which is similar to the expression (3.1) obtained in [14] for the theta scheme. For the iterations to converge \( |A| < 1 \), otherwise the imposed interface boundary conditions must be interchanged. It is reiterated that the expression in (6.24) is equal to the ratio of thermal effusivities of the coupled domains, i.e. \( |A| = \sigma = \frac{\alpha_1}{\alpha_2} \). Therefore, for stability (\( |A| < 1 \)), the domain with the higher \( \sigma \) is assigned the Neumann condition and the one with the lower \( \sigma \) the Dirichlet condition.

Based on (6.24), it is observed that for the Dirichlet-Neumann formulation, the rate of convergence of Gauss-Seidel interface iterations is fast when the thermal interaction between the subdomains is weak \( \sigma \ll 1 \), and decreases as the strength of the interaction increases \( \sigma \rightarrow 1 \). For strongly coupled problems, more robust and efficient iteration methods to increase the rate of convergence of the iterations should be used, the simplest of which is the use of a fixed under-relaxation in the iterations. Following the steps in Henshaw and Chand [14], an analytical estimate of the optimum value of the under-relaxation is given by:

\[ \omega_{opt} = \frac{1}{1 + |A|}, \quad (6.25) \]
6.2. Numerical Examples

where $A$ is given by (6.22). In the results section, to increase the rate of convergence of the iterations, we consider the Aitken method (where the value of the under-relaxation is not fixed and may vary during the iterations), and compare the results with the estimate provided by (6.25). For the details of the Aitken algorithm, the reader is referred to [24] and for more advanced techniques to expedite the rate of convergence of the interface iterations see for example [9].

6.2 Numerical Examples

In this section, the strongly-coupled partitioned algorithm is used to solve a conjugate heat transfer problem in order to demonstrate the applicability of the method, to validate the performed analytical stability analysis, and to investigate the computational efficiency of the algorithm relative to lower order time integration schemes and the high order loosely-coupled IMEX schemes.

6.2.1 Problem description and specifications

As a test-case, the unsteady conjugate natural convection in a square enclosure presented in section 4.5 is considered. In order to investigate the influence of the strength of the thermal interaction on the rate of convergence of the iterations, the test-case is solved using the following two sets of parameters:

**Case-a**

\[
\begin{align*}
k_1 &= 1600, & \rho_1 &= 7500, & c_{p,1} &= 0.5, \\
k_2 &= 1, & \rho_2 &= 1, & c_{p,2} &= 1, & \nu_2 &= 0.7, & \beta &= 0.01, & g &= 0.7 \cdot 10^7, \\
L &= 1, & h &= 0.2, & T_{ref} &= 1, & T_H &= 2, & T_C &= 1, \\
\frac{k_1}{k_2} &= 1600, & \frac{\alpha_1}{\alpha_2} &= 0.4, & Pr &= 0.7, & Ra &= 1 \cdot 10^5,
\end{align*}
\] (6.26)

**Case-b**

\[
\begin{align*}
k_1 &= 80, & \rho_1 &= 7.5, & c_{p,1} &= 0.12, \\
k_2 &= 1, & \rho_2 &= 1, & c_{p,2} &= 1, & \nu_2 &= 7, & \beta &= 0.01, & g &= 4.9 \cdot 10^7, \\
L &= 1, & h &= 0.2, & T_{ref} &= 1, & T_H &= 2, & T_C &= 1, \\
\frac{k_1}{k_2} &= 80, & \frac{\alpha_1}{\alpha_2} &= 88.9, & Pr &= 7, & Ra &= 7 \cdot 10^4,
\end{align*}
\] (6.27)

The ratio between the material properties of the coupled domains in (6.26) and (6.27) correspond to those of steel-air and steel-water couplings respectively. The thermal interaction between the coupled domains is weak ($\sigma = 4.1 \cdot 10^{-4} \ll 1$) for **Case-a**, and relatively strong for **Case-b** ($\sigma = 0.1$).

Based on the prescribed values of the material properties (in both **Case-a** and **Case-b**), for stability $\Omega_2$ takes the Dirichlet condition at the interface, while $\Omega_1$ the Neumann condition.
6.2.2 Solution procedure

The solid domain \( \Omega_1 \) is discretized using the finite volume method with the temperature stored in the cell center. The fluid domain \( \Omega_2 \) is also discretized using the finite volume method with staggered arrangement of the variables \([44]\). In each of the subdomains, a uniform grid-spacing is used in both directions: for the solid domain: \( N_{1,x} = 80, N_{1,y} = 20 \) with \( N \) number of cells, and for the fluid domain \( N_{2,x} = 80, N_{2,y} = 80 \). Noting that \( \Omega_1 \) does not have a node at the interface as result of the cell-centered discretization, linear extrapolation from the cells in \( \Omega_1 \) close to the interface is used to approximate the interface temperature (see section 3.2 for more details). In both the momentum and energy equations, the second order centered scheme is used for discretizing the convective terms and the second order central differencing scheme is used to discretize the diffusive terms. In the flow solver, at each (implicit) stage, Picard iterations are used for solving the non-linear coupled equations \([44]\). The flow solver is iterated to a strict tolerance \( \epsilon_{\text{iter}} < 10^{-9} \), \( \epsilon_{\text{iter}} \): maximum of the residuals of the momentum and energy equations to eliminate iteration error as a contaminating variable in the study; the residual \( R_w^\phi \) at each iteration \( w \) is computed using,

\[
R_w^\phi = -\frac{\phi^w - \phi^n}{\Delta t a_{k,k}} + \mathcal{F}_\phi^w + \frac{1}{a_{k,k}} \sum_{i=1}^{k-1} a_{k,i} \mathcal{F}_{\phi}^{(i)},
\]

(6.28)

where \( \phi \) denotes the velocity and temperature fields. Furthermore, the linear systems in the flow and solid solvers are solved to machine precision.

6.2.3 Stability

The CHT problem is solved for Case-a and Case-b using the strongly-coupled algorithm. The four-stage third order ESDIRK (ESDIRK-3) is used for time integration (note that the first stage is explicit). Simulations are run to \( t_{\text{final}} = 0.01 \) using \( \Delta t = 5 \cdot 10^{-4} \). For Case-b, computations are performed starting from an initial temperature field of unity imposed on the global domain: \( T(x,t=0) = 1 \) for \( x \in \Omega = \Omega_1 \cup \Omega_2 \). For Case-a, initially computations are carried out with the monolithic ESDIRK-3 (from an initial temperature field of unity imposed on the global domain) to time level of \( t_{\text{IC}} = 3 \cdot 10^{-2} \) using a time step of \( \Delta t_{\text{IC}} = 5 \cdot 10^{-4} \). The obtained solution is used as initial condition for the partitioned computations. For each case, an average rate of convergence of iterations per stage of the ESDIRK, \( \Phi_{\text{comp}}^{(k)} \), is computed using,

\[
\Phi_{\text{comp}}^{(k)} = \left( \frac{\| r_N^J \|}{\| r_0^J \|} \right)^{\frac{1}{J}},
\]

(6.29)

where \( r_j \) denotes the interface residual at iteration \( j \), and \( r^0 \) is the interface residual after the first implicit solve (at each stage). For BGS-12, \( r^J = |q_1(I)^J - q_1(I)^{J-1}| \).
The max-norm is used in the evaluation of norms of the residuals. Interface iterations are performed at each stage until \( \| r^N \| < 10^{-9} \). To present the results in Table 6.1, for each stage, \( \Phi^{(k)}_{\text{comp}} \) is averaged over the 20 time steps. The computed values of convergence rate are compared with the estimate \( \Phi^{(k)}_{\text{est}} \) obtained from the stability analysis, (6.24).

**Table 6.1:** Rate of convergence of interface iterations at each stage of ESDIRK-3

| Case  | \( \Phi^{(k)}_{\text{est}} \) | \( \Phi^{(k)}_{\text{comp}} \) |
|-------|----------------|-----------------|----------------|----------------|
|       | stage - 2     | stage - 3       | stage - 4 |
| Case-a| 4.1 \cdot 10^{-4} | 3.0 \cdot 10^{-4} | 3.0 \cdot 10^{-4} | 3.0 \cdot 10^{-4} |
| Case-b| 0.12 \cdot 10^0  | 0.91 \cdot 10^{-1} | 0.91 \cdot 10^{-1} | 0.91 \cdot 10^{-1} |

As the results show, \( \Phi^{(k)}_{\text{est}} \) provides a good estimate of the rate of convergence of subiterations for each stage of the ESDIRK. Furthermore, for each case, it is observed that \( \Phi^{(k)}_{\text{comp}} \) is almost the same for all stages due to the equality of the diagonal coefficients of the stages in the ESDIRK schemes and the minimal influence, if any, of the previous time step and the summation of the previously evaluated stage residuals.

Similar computations were also carried out using the Aitken relaxation in which the value of the under-relaxation is computed at each iteration according to (see [24] for the complete algorithm):

\[
\omega^j = -\omega^{j-1} \frac{(r^j - r^{j-1})^T(r^j - r^{j-1})}{\| r^j - r^{j-1} \|^2_2} \tag{6.30}
\]

As the results in Table 6.2 demonstrate, the Aitken relaxation method improves the rate of convergence of the interface iterations. While for Case-a, the under-relaxation remained constant within all the subiterations, for Case-b, it varied within the iterations in each stage. The presented value of the computed under-relaxation factor \( \omega_{\text{comp}} \) is obtained by averaging over the corresponding values of all the performed iterations within the 20 time-steps. The results in the table also show that the computed value of the under-relaxation \( \omega_{\text{comp}} \) is in good agreement with the analytical estimate of the optimum value \( \omega_{\text{est}} = \frac{1}{1 + \Phi^{(k)}_{\text{est}}} \).

To investigate whether the Aitken relaxation more effectively reduces the number of iterations relative to a fixed value of under-relaxation, for Case-b similar computations were carried out using the fixed under-relaxation of \( \omega_{\text{est}} = 0.89 \). The average of the computed rates of convergence for each stage is approximately \( 0.5 \cdot 10^{-1} \); using the Aitken method increases the rate of convergence by a factor of 2.5.
Table 6.2: Influence of under-relaxation on the rate of convergence of iterations.

<table>
<thead>
<tr>
<th>Case</th>
<th>$\Phi_{est}^{(k)}$</th>
<th>$\Phi_{comp}^{(k)}(\omega)$</th>
<th>$\omega_{est}$</th>
<th>$\overline{\omega}_{comp}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case-a</td>
<td>$4.1 \cdot 10^{-4}$</td>
<td>$3.4 \cdot 10^{-6}$</td>
<td>$1.6 \cdot 10^{-6}$</td>
<td>$1.6 \cdot 10^{-6}$</td>
</tr>
<tr>
<td>Case-b</td>
<td>$0.12 \cdot 10^0$</td>
<td>$0.2 \cdot 10^{-1}$</td>
<td>$0.2 \cdot 10^{-1}$</td>
<td>$0.2 \cdot 10^{-1}$</td>
</tr>
</tbody>
</table>

### 6.2.4 Accuracy and efficiency assessment

When the thermal interaction between the subdomains is weak ($\sigma \ll 1$), as demonstrated in Chapter 5 the loosely-coupled IMEX schemes provide an efficient way of solving time-accurate CHT problems. As the thermal interaction between the domains becomes stronger ($\sigma \rightarrow 1$), the stability and the temporal accuracy of the loosely-coupled IMEX schemes reduce compared to the monolithic approach. As a result, smaller time-steps are required to lower the partitioning error (which consequently increases the accuracy of the partitioned solution and/or stabilizes the partitioned algorithm). Under such cases, as an alternative, the strongly-coupled ESDIRK schemes (strongly-coupled algorithm with ESDIRK schemes for time integration) can be used where the partitioning error is reduced by performing interface iterations. Therefore, while the strongly-coupled algorithm performs more interface iterations per stage compared to a single one in the loosely coupled IMEX schemes, for the same time-step size, it generally provides temporally more accurate solutions (assuming that the loosely-coupled algorithm is stable). In this section, we investigate whether the additional work per time step is compensated by the gain in accuracy and stability. In addition, computational efficiency relative to the strongly-coupled Crank-Nicolson is also analyzed.

Computations are carried out for Case-b where the thermal interaction between the subdomains is relatively strong. Initially the global domain is set to a temperature of unity: $T(\mathbf{x}, t = 0) = 1$ for $\mathbf{x} \in \Omega = \Omega_1 \cup \Omega_2$. Then, computations are carried out with the monolithic approach of Schäfer and Teschner [38] (a single temperature equation is solved across both the subdomains while using a separate flow field solver in the fluid subdomain) to time level $t_{IC} = 1 \cdot 10^{-4}$, in order to step over the time that is required for the heat (thermal penetration depth) to travel from the bottom boundary to the interface (thermal interaction between the two subdomains has been initiated at this time). The fifth order ESDIRK (ESDIRK5) with time step-size of $\Delta t_{IC} = 2 \cdot 10^{-5}$ is used for time integration. The obtained solution at $t_{IC}$ is used as initial condition for the problem.

The coupled problem is advanced in time to $t_{final} = 0.02$ using the strongly-coupled algorithm, as well as the loosely-coupled algorithms of Chapter 4 (predictor-corrector Crank-Nicolson) and Chapter 5 (loosely-coupled IMEX). For each case, the partitioned solution at $t_{final}$ was compared to that of the temporally exact solution (defined as the monolithic solution at $t_{final}$ obtained using a fine time-step size: $\Delta t_{final} = 2 \cdot 10^{-5}$).
ESDIRK5 is used for time integration with $\Delta t_{\text{fine}} = 2 \cdot 10^{-5}$). To investigate how well the coupled problem is solved compared to the monolithic approach, computations are also carried out with the monolithic solver.

Again, we review several definitions which will be used in the discussion that follows. The time integration error ($\epsilon_t$) is defined as the difference between the temporally exact solution and the monolithic solution at $t_{\text{final}}$ obtained with a certain time step which is coarser relative to $\Delta t_{\text{fine}}$. The difference between the temporally exact solution and the partitioned solution at $t_{\text{final}}$ is defined as the total error of the partitioned solution ($\epsilon_{\text{total}}$) and represents the sum of the time integration error ($\epsilon_t$) and partitioning error ($\epsilon$), ($\epsilon_{\text{total}} = \epsilon_t + \epsilon$). For $\epsilon_{\text{total}}$ to be of the same order as $\epsilon_t$, the partitioning error $\epsilon$ needs to be at least of the same order as $\epsilon_t$.

### 6.2.4.1 Temporal accuracy

In Fig. 6.1, the total error in the solution fields obtained with the loosely-coupled algorithms, integrating $\Omega_1$ first (BGS-12), is shown as a function of time step size. Also shown, is the corresponding (time integration) error in solution field obtained using the monolithic approach.

For a time-accurate partitioned solution, the partitioning error ($\epsilon$) should be as low as possible, desirably below the time integration error such that the partitioning error is not the dominant source of error in the partitioned solution (hence $\epsilon_{\text{total}} \approx \epsilon_t$). However, as Fig. 6.1a demonstrates, due to the strong thermal interaction, the accuracy of the temperature field obtained using the IMEX schemes is low relative to their monolithic solutions. In addition, the temporal convergence character of the total error of the temperature field is also influenced by the partitioning error; to observe the full-design orders smaller time-step sizes need to be considered. Furthermore, it is observed that as the order of the time integration scheme increases, the deviation of the partitioned solution from its corresponding monolithic solution increases. Similar observations can be made for the convergence of the total error in the $x$-component of the velocity field as shown in Fig. 6.1b. However, there is a weaker influence of partitioning on the temporal accuracy and convergence character of the total error in the velocity field compared to the temperature field.

The stability of the IMEX schemes in solving this CHT problem was considered numerically in Chapter 5. The approximate $\Delta t$ at which simulations become unstable for each of the time integration schemes is shown in Table 5.3. Due to the relatively strong thermal interaction between the subdomains, the choice of $\Delta t$ using the IMEX schemes is restricted by stability rather than accuracy. The restriction will be higher as $\sigma \to 1$.

In Fig. 6.2a, the total error in the global temperature field obtained using the strongly-coupled algorithm (with $BGS - 12$) is shown as a function of $\Delta t$ for several time integration schemes. In the first subiteration of each stage (iteration $j = 0$), the IMEX predictor (5.2) is used for the approximation of the coupling term. For
Figure 6.1: Total error in (a) global temperature field and (b) $x$-component of the velocity as a function of $\Delta t$, using the loosely coupled algorithms. In the figures, $CN_{\text{mono}}$ refers to monolithic solution obtained with Crank-Nicolson, $\text{ESDIRK(3-5)mono}$ refer to the monolithic solutions obtained using the $3^{rd}$-$5^{th}$ order ESDIRK schemes. The partitioned solution obtained using the predictor-corrector Crank-Nicolson scheme is denoted by $\text{pred-corr CN}$, and the partitioned solutions obtained using the $3^{rd}$-$5^{th}$ order IMEX schemes are denoted by $\text{IMEX(3-5)}$.

Figure 6.2: Total error in (a) global temperature field and (b) $x$-component of the velocity as a function of $\Delta t$, using the strongly-coupled algorithm. Results of the Crank-Nicolson scheme are denoted by $CN$ (3 Sub) where Sub indicates the number of subiterations per time-step. Results of the ESDIRK schemes are denoted by $\text{ESDIRK(3-5) (2 Sub)}$ where Sub indicates the number of subiterations per stage.

the ESDIRK schemes, performing two subiterations at each stage was found to be sufficient (based on numerical experiments) for obtaining stable solutions using
time-steps which were found to be unstable for the IMEX schemes (1 interface iteration per stage). When the Crank-Nicolson scheme is used for time integration, 3 subiterations at each time-step were necessary. No under-relaxation was used in the computations ($\omega = 1$). As Fig. 6.2a demonstrates, as long as the partitioning error is above the time integration error, interface iterations improve the temporal accuracy of the partitioned solution. Similar observations can be made for the convergence of the total error of the $x$-component of the velocity field with $\Delta t$ as shown in Fig. 6.2b.

6.2.4.2 Computational efficiency

In order to compare the computational work of the strongly-coupled ESDIRK algorithm with the loosely-coupled IMEX, the total error in the temperature field and $x$-component of the velocity field are plotted against the work in respectively Fig. 6.3a and Fig. 6.3b. The work ($W$) is defined as the total number of interface iterations ($\phi$) to reach $t_{final}$, $W = \frac{\phi t_{final}}{\Delta t}$.

![Figure 6.3: Comparison of the computational work of the loosely-coupled and strongly-coupled algorithms using respectively IMEX and ESDIRK schemes (for time integration) for obtaining the solution to: Fig. 6.3a the temperature field, Fig. 6.3b $x$-component of the velocity.](image)

For levels of accuracy for which the loosely-coupled IMEX schemes are unstable, the strongly coupled ESDIRK schemes are obviously more efficient. By comparing the work of two partitioned algorithms for the accuracy range in which the IMEX schemes are stable, and with reference to figures Fig. 6.1 and Fig. 6.2, it is noted that performing interface iterations is computationally more efficient than lowering the time-step size using the loosely-coupled IMEX; the gain in temporal accuracy (as a result of lowering the partitioning error with iterations) outweighs the additional work per stage relative to the IMEX schemes. Furthermore, once the partitioning er-
ror has been driven below the time integration error, performing interface iterations does not increase the accuracy of the solution, but does increase the computational work.

Prior to comparing the computational efficiency of the ESDIRK schemes with Crank-Nicolson, as an illustration of the quality of the solution at different error levels, the time-history of the temperature at the interface and \( x \)-component of the velocity at the center of the cavity is demonstrated in Fig. 6.4-Fig. 6.5. As reference, the data from the temporally exact solution are also included. Since the Crank-Nicolson scheme is not L-stable, as Fig. 6.4a demonstrates, the interface temperature exhibits an oscillatory behavior in time for time-steps which are larger than the time-decay of the rapid transients in the solution. While the velocity does not demonstrate such oscillations, however, the accuracy is influenced by the temperature oscillations in particular for the large time step sizes.

The ESDIRK schemes on the other hand are L-stable and as Fig. 6.5 shows, such oscillatory behavior does not occur. It is noted that in unsteady CHT problems, the temporal variations of the interface temperature \( (T_I(t)) \) and interface heat flux \( (q_I(t)) \) are important quantities of interest, and their accurate resolution is necessary. Therefore, we continue the discussion, analyzing the computational efficiency in solving the temperature field.

![Figure 6.4: Time-history of (a) the interface temperature and (b) \( x \)-component of the velocity at the center of the square enclosure using Crank-Nicolson for time integration.](image)

The total error in the temperature field is plotted against the work in Fig. 6.6a. A time-step size approximately in the range of \( 5 \cdot 10^{-4} \leq \Delta t \leq 1 \cdot 10^{-3} \) seems to be sufficient to capture the transients with reasonable accuracy using the Crank-Nicolson scheme (as Fig. 6.4a shows). The temporal accuracy of temperature field using a time-step size in this range is approximately \( 1 \cdot 10^{-3.8} \leq e_{total}^{T} \leq 1 \cdot 10^{-3.2} \). Using ESDIRK4 with two subiteration per stage, reduces the computational work to obtain an accuracy in this range by approximately a factor of \( 1.3 - 1.8 \).
6.2. Numerical Examples

Figure 6.5: Time-history of (a) the interface temperature and (b) $x$-component of the velocity at the center of the square enclosure using the fourth order time integration.

computational efficiency is higher for higher accuracies.

Figure 6.6: Computational work of several time integration schemes for obtaining the solution to: (a) the temperature field, (b) $x$-component of the velocity, using the strongly-coupled algorithm.

While the BDF2 scheme was not considered for the partitioned solution of the CHT problem, however, the computational efficiency of the ESDIRK schemes was compared to BDF2 in solving the coupled problem monolithically. As the results in Fig. 6.7 show, the ESDIRK schemes are more efficient than the BDF2 scheme for reasonable accuracy levels.
6.3 Conclusions

In order to reduce the computational work of solving time-accurate conjugate heat transfer problems, we considered the use of high order implicit time integration schemes which have the potential to improve the computational efficiency relative to the commonly used second order implicit schemes. For strongly coupled problems, we presented a strongly-coupled solution algorithm where the high order L-stable ESDIRK schemes are used to advance the solution in time within each separate fluid and solid subdomains.

The stability and rate of convergence of performing (Gauss-Seidel) subiterations at each stage of the ESDIRK schemes were analyzed. Dirichlet-Neumann interface conditions were used for spatial coupling between the subdomains. Based on the stability analysis, the domain with the higher effusivity is assigned the Neumann condition and the one with the lower effusivity the Dirichlet condition. Furthermore, the interface iterations converge with a rate approximately given by the ratio between the thermal effusivities of the coupled domains ($\sigma$). For weakly coupled problems, $\sigma \ll 1$, subiterations converge rapidly. However, as the strength of the thermal interaction increases (as $\sigma \to 1$), the convergence rate of the iterations decreases, and more robust and efficient subiteration methods such as the Aitken under-relaxation should be used to increase the rate of convergence of the iterations.

The results obtained by solving a numerical example (an unsteady conjugate natural convection in an enclosure), showed good agreement with the performed analytical stability analysis.

Furthermore, the (computational) work-(temporal) precision character of several schemes in solving a strongly-coupled CHT test-case was compared over a range
of accuracy requirements. From the efficiency investigation it was observed that performing subiterations with the strongly-coupled ESDIRK algorithm was more efficient than lowering the time-step size using the loosely-coupled IMEX algorithm. In addition, by using the ESDIRK schemes, gain in computational efficiency relative to Crank-Nicolson was observed for time-accurate solutions (a factor of 1.8 using ESDIRK4). The computational gain was higher for smaller tolerances.
Chapter 7

High order ESDIRK schemes and collocated finite volume discretization of unsteady incompressible flows

V. Kazemi-Kamyab, A.H. van Zuijlen, H. Bijl: Analysis and application of high order implicit Runge-Kutta schemes to collocated finite volume discretization of the incompressible Navier-Stokes, Submitted.

For the (loosely and/or strongly coupled) partitioned algorithms to preserve the temporal design order, it is necessary for the separate physics solvers to have the correct order behavior for the uncoupled simulations. In this chapter, the application of the high order ESDIRK schemes (3$^{rd}$ - 5$^{th}$ order) to cell-centered collocated finite volume discretization of incompressible flows is considered. The focus of the chapter is on the development of a segregated solution algorithm which will preserve the temporal design order of the multi-stage ESDIRK schemes on this spatial discretization.

7.1 Introduction

The unsteady incompressible Navier-Stokes equations in primitive variables are given by:

\[
\frac{\partial \mathbf{u}}{\partial t} = -\nabla \cdot (\mathbf{uu}) + \nu \nabla^2 \mathbf{u} - \nabla p = \mathbf{R}(\mathbf{u}) - \nabla p = \mathcal{F}(\mathbf{u}, p, t),
\]

\[
\nabla \cdot \mathbf{u} = 0.
\]
where $\mathbf{u}$ is the velocity vector, $p$ is the kinematic pressure and $\nu$ the kinematic viscosity. The stability and accuracy of a numerical approach to solve (7.1) in primitive variables, are influenced by the method with which the velocity-pressure coupling is resolved; both in the solution algorithm and in the arrangement of the variable [28].

In engineering applications, typically a fully implicit time integration is preferred over an explicit one in order to circumvent time step restrictions due to probable stiffness in the problem. Furthermore, as a potential solution to reduce the cost of performing transient computations, high order implicit time integration schemes can be employed in place of the commonly used second order Crank-Nicolson and second order backward difference (BDF2) schemes. For example, in [41] computational efficiency of a class of high order multi-stage time integration schemes, Rosenbrock–Wanner (ROW), relative to Crank-Nicolson is demonstrated for an incompressible flow test-case. An inf–sup stable ($Q_2/P_1$) finite element method is used for spatial discretization and the algebraic system of the fully discretized INS equations is solved directly (i.e. a segregated solution method is not used). Another example can be found in [1], for a compressible flow test-case, where the computational efficiency of high order ESDIRK schemes relative to BDF2 has been demonstrated.

A concern in the application of high order time integration schemes to the unsteady INS equations is the possibility of temporal order reduction due to the spatial discretization, and/or the solution algorithm. In this chapter, this issue is addressed by applying high order ESDIRK schemes to the cell-centered collocated finite volume discretization of the INS equations, and using a segregated solution algorithm to solve the resultant fully discretized equations.

It is well known that a standard collocated grid finite volume method has convergence problems and spurious oscillations in the pressure field can occur which deteriorate the solution [18, 28]. The checker-board pressure field arises as result of centered discretization of the continuity equation and the pressure gradient in the momentum equation [18, 28]. A widely used method in the literature and CFD packages which tackles this problem is the interpolation procedure proposed by Rhie and Chow [35]. The basic mathematical principle of this method is to suppress the spurious pressure modes by perturbing the continuity equation with a pressure regularization (dissipation) term [44]. In this approach discretized momentum equations are formulated for the convective (or face) velocities which appear in the discrete continuity equation [28]. The result of the interpolation technique is an expression for the convective velocity which consists of the standard linear interpolation of the cell-centered velocities with the addition of a pressure smoothing term [8, 18, 26]. It can be shown, using some assumptions, that the pressure smoothing term is a third order artificial dissipation term, which accordingly results in the introduction of a fourth order dissipation term in the continuity equation [18, 26]. In addition, since the face velocity enters the convective flux of the momentum equation, the interpolation also introduces a fourth-order smoothing term into the momentum equation [26].
A defect of this interpolation procedure introduced for steady-state computations is that its extension to unsteady flow conditions is not obvious [26]. In computing the solution to the unsteady INS equations (in particular using a class of segregated solution algorithms such as SIMPLE-like and PISO-like approaches), care should be taken in selecting the interpolation method, otherwise it will result in a time-step dependent steady-state solution, temporal order reduction, and/or temporal inconsistency. Reviews of the literature on this topic are presented in [8] and [33]. For the first order Backward Euler (BDF1), to the author’s knowledge, currently a few time-consistent interpolation schemes are available in the literature; they are the interpolation schemes proposed by Lien and Leschziner [26] (and later Yu et al. [47]), Cubero and Fueyo [8], and Pascau [33]. It follows that in applying high order implicit time schemes, one of the three interpolation procedures should be adopted. Yet, additional considerations might be required in order to preserve temporal consistency and/or order of higher order schemes. For example, for the commonly used second order schemes these issues have been addressed and studied in [8, 42, 47]. In this chapter, a face velocity interpolation procedure which preserves the temporal design order of the high order multi-stage ESDIRK schemes is introduced. In addition, the details of an iterative pressure-based time advancing algorithm comprising the designed interpolation method are discussed.

In what follow, first the semi-discrete form of (7.1) is obtained by discretizing the spatial operators. After a brief discussion on high order ESDIRK schemes, the details of a corresponding temporally order-preserving face-velocity interpolation method is presented. This is followed by discussing the solution algorithm. Next, numerical examples are used to investigate the temporal order preservation of the algorithm.

7.2 Spatial discretization and semi-discrete form

The method of lines [25] is used to discretize (7.1), with spatial operators being discretized first to obtain the semi-discrete form of the equations. The cell-centered finite volume approach is considered for spatial discretization with collocated arrangement of the primitive variables. The computational domain is subdivided into finite volumes (or cells) where each cell is bounded by arbitrary number of cell faces. The volume integral form of (7.1) is applied to each finite volume, and the Gauss divergence theorem is used to convert the volume integrals to surface integration over the closed boundary of the cell (see [17, 42] for more details). The resultant discrete form of (7.1) is give by:

$$ V_P \frac{dU_P}{dt} = - \sum_f \phi_f U_f + \nu \sum_f (\nabla U)_f \cdot n_f S_f - \sum_f p_f n_f S_f, \quad (7.2) $$

$$ \sum_f U_f \cdot n_f S_f = 0. \quad (7.3) $$
where the subscripts \( P \) and \( f \) represent the cell-center and face-center values (see Fig. 7.1). \( V_P \) is the volume of the cell, and for a given cell face \( f \), \( \mathbf{n}_f \) is the face normal vector, and \( S_f \) is its surface area. The convective velocity through the face is denoted by \( \mathbf{U}_f \), and \( \phi_f = \mathbf{U}_f \cdot \mathbf{n}_f S_f \) is the volumetric flow rate through the face.

![Figure 7.1: Geometric sketch of a control volume and its neighboring cell.](image)

After using appropriate schemes to discretize the spatial operators, the following semi-discretized form of (7.1) for each cell \( P \) is obtained (where (7.2) is divided by the cell volume):

\[
\frac{dU_P}{dt} + a_P U_P - \sum_{N=nb(P)} a_N U_N = - (\nabla p)_P + r_P, \quad (7.4)
\]

\[
\sum_{f} \phi_f = 0 \quad (7.5)
\]

where \( a_P \) and \( a_N \) are the diagonal and off-diagonal coefficients of the (spatial) discretization matrix. \( r_P \) includes parts of convection and diffusion terms treated explicitly, as well as boundary contributions. The term \( (\nabla p)_P \) denotes the (average) pressure gradient at \( P \), \( (\nabla p)_P = \frac{1}{V_P} \sum_{f} \frac{N_f}{P} p_f \mathbf{n}_f S_f \) (Green-Gauss gradient reconstruction). The pressure at the face is evaluated using linear interpolation of the adjacent cell-centered values. Using the following definition:

\[
H_P(U) = \sum_{N=nb(P)} a_N U_N + r_P, \quad (7.6)
\]

we can rewrite the semi-discretized form of the momentum equation in (7.4) as:

\[
\frac{dU_P}{dt} + a_P U_P = H_P - (\nabla p)_P. \quad (7.7)
\]

By defining the residual vector \( \mathbf{F}_P \) as,

\[
\mathbf{F}_P = -a_P U_P + H_P - (\nabla p)_P, \quad (7.8)
\]

equation (7.7) can be expressed by,

\[
\frac{dU_P}{dt} = \mathbf{F}_P(U, p, t). \quad (7.9)
\]
7.3 Time integration

The high order ESDIRK schemes (discussed in section 3.3) are considered for time integration. For an ODE system of the form $\frac{dU}{dt} = \mathbf{F}(\mathbf{U}, \mathbf{p}, t)$, the solution at each stage of the ESDIRK scheme can be written as:

$$\frac{U_P^{(k)} - U_P^n}{\Delta t} = \sum_{i=1}^{k} a_{ki} \mathbf{F}(U^{(i)}, p^{(i)}, t^n + c_i \Delta t), \quad (7.10)$$

or,

$$\frac{U_P^{(k)} - U_P^n}{a_{kk} \Delta t} = \mathbf{F}_P^{(k)} + \frac{1}{a_{kk}} \sum_{i=1}^{k-1} a_{ki} \mathbf{F}_P^{(i)}, \quad (7.11)$$

where $a_{ki}$ are the stage weights (with $a_{kk} = \gamma$), and $c_i = \sum_j a_{ij}$ are the quadrature nodes of the scheme, $t^{(i)} = t^n + c_i \Delta t$. The solution at the next time level is obtained by,

$$U^{n+1}_P = U^n_P + \Delta t \sum_{i=1}^{s} b_i \mathbf{F}_P^{(i)} , \quad (7.12)$$

where $b_i$ are the scheme’s main weights with $\sum_i b_i = 1$, and $s$ is the number of stages. In this paper, stiffly accurate ESDIRK schemes are considered where $a_{si} = b_i$ and thus the solution of the last stage is equal to the solution of the next time-level, $U^{n+1}_P = U^{(s)}_P$. Therefore, computing (7.12) becomes unnecessary. Since the ESDIRK schemes have reduced stage orders, they are susceptible to order-reduction in the presence of substantial stiffness (see [3]).

7.4 Face-velocity interpolation

In order to avoid pressure-velocity decoupling, the method proposed by Rhie and Chow [35] is followed here; rather than evaluating the convective velocities $U_f$ from a direct interpolation of the neighboring cell-center nodes, discretized momentum equation for the convective velocities are constructed. For unsteady flow computation with BDF1 for time integration, there are a few time-consistent interpolation schemes available in the literature as discussed in the introduction. Here, the approach of Lien and Leschziner [26] (or Yu et al. [47]) is adopted to evaluate the appropriate terms in the discretized momentum equation formulated for the face-velocity.

As (7.11) shows, from an implementation view point, each stage of the ESDIRK scheme resembles the BDF1 scheme with a source term ($\frac{1}{a_{ki}} \sum_{i=1}^{k-1} a_{ki} \mathbf{F}_P^{(i)}$). We will proceed with deriving an equation for the face velocity with particular emphasis on the treatment of the source term (which arises from time discretization) such that the design order of the ESDIRK schemes is preserved.
Applying the ESDIRK schemes to the semi-discrete form of the momentum equation (7.7), we arrive at (with reference to (7.11)),

\[
\tilde{a}_P U_p^{(k)} = \frac{1}{\Delta t_{akk}} U_n^p - (\nabla p)_P^{(k)} + H_P^{(k)} + \frac{1}{a_{kk}} \sum_{i=1}^{k-1} a_{ki} F_P^{(i)},
\]

(7.13)

where,

\[
\tilde{a}_P = \frac{1}{\Delta t_{akk}} + a_P.
\]

(7.14)

Dividing (7.13) by \(\tilde{a}_P\), yields the equation for the cell-center velocity:

\[
U_p^{(k)} = \frac{1}{\Delta t_{akk}} U_n^p + \frac{H_P^{(k)}}{\tilde{a}_P} - \frac{(\nabla p)_P^{(k)}}{\tilde{a}_P} + \frac{1}{a_{kk}} \sum_{i=1}^{k-1} a_{ki} F_P^{(i)}.
\]

(7.15)

An equivalent equation as the one for the centered velocity (7.15) can be defined for the face (convective) velocity:

\[
U_f^{(k)} = \frac{1}{\Delta t_{akk}} U_n^f + \frac{H_f^{(k)}}{\tilde{a}_f} - \frac{(\nabla p)_f^{(k)}}{\tilde{a}_f} + \frac{1}{a_{kk}} \sum_{i=1}^{k-1} a_{ki} F_f^{(i)}.
\]

(7.16)

where \((\nabla p)_f\) denotes the face pressure gradient normal to the surface \(f\). On a cartesian grid, the gradient is computed using the central differencing scheme. Following Lien and Leschziner [26], \(H_f\) and \(\tilde{a}_f\) are approximated by the following interpolations:

\[
H_f = [H_P]_f,
\]

(7.17)

\[
\tilde{a}_f = [\tilde{a}_P]_f,
\]

(7.18)

where the symbol \([\zeta]_f\) denotes linear interpolation of the cell-centered values encompassing the face \(f\). To retain the temporal consistency of the method, \(H_P\) in (7.6) only contains contributions as a result of the discretization of the spatial operators, and does not include the previous time-step solution of the cell-centered velocity \(U_P^n\) [8,26,33].

The face residual vector \(F_f\) is evaluated by considering the fully-discretized form of \(\frac{dU_f}{dt} = F_f\):

\[
\frac{U_f^{(k)} - U_f^n}{\Delta t_{akk}} = F_f^{(k)} + \frac{1}{a_{kk}} \sum_{i=1}^{k-1} a_{ki} F_f^{(i)}.
\]

(7.19)

Noting that at the end of a stage \(U_f^{(k)}\) is known, it is possible to evaluate \(F_f^{(k)}\) using:

\[
F_f^{(k)} = \frac{U_f^{(k)} - U_f^n}{\Delta t_{akk}} - \frac{1}{a_{kk}} \sum_{i=1}^{k-1} a_{ki} F_f^{(i)}.
\]

(7.20)
7.5. Solution algorithm

The (cell-center) pressure is evaluated by transforming the discrete continuity equation (7.3) into an equation for pressure. Substituting (7.16) into (7.3) (assuming that $U_f^{(k)}$ is divergence free), yields:

$$\sum_f \left( \frac{1}{a_f} (\nabla p)_f \right) \cdot n_f S_f = \sum_f \left( \frac{1}{\Delta t a_{kk}} \frac{U^n_j}{a_f} + \frac{H_f}{a_f} + \frac{1}{a_{kk}} \sum_{i=1}^{k-1} a_{ki} F_f^{(i)} \right) \cdot n_f S_f. \quad (7.21)$$

By rewriting (7.13) as an equation for $H_P$, and substituting it into (7.16), and by noting (7.17), an equivalent equation for the face velocity is obtained:

$$U_f^{(k)} = \left[ \tilde{a}_P U_P^{(k)} \right]_f - \frac{(\nabla p)_f^{(k)} - [ (\nabla p)_P^{(k)} ]_f}{\tilde{a}_f} + \frac{1}{\Delta t a_{kk}} \frac{U^n_j - [U^n_P]_f}{\tilde{a}_f}$$

+ $\frac{1}{a_{kk}} \sum_{i=1}^{k-1} a_{ki} F_f^{(i)} - \left[ \sum_{i=1}^{k-1} a_{ki} F_p^{(i)} \right]_f,$ \quad (7.22)

where $\tilde{a}_f$ is evaluated by (7.18). By noting that at steady-state, $U_m^{n+1} = U_m^{(k)} = U_m^n$, and $F_m = 0$ (with $m = P$ or $f$), (7.22) reduces to the following form:

$$U_f = \left[ a_P U_P \right]_f - \frac{(\nabla p)_f - [(\nabla p)_P]_f}{a_f} \quad (7.23)$$

Therefore, the steady state solution is independent of $\Delta t$ and the residual vectors $F_P$ and $F_f$.

7.5 Solution algorithm

There are several routes available for advancing the solution to the unsteady INS equations in time, of which the pressure or pressure correction methods (also including the non-iterative fractional step or projection methods) are currently the most commonly used approaches [5,26]. These methods allow the system to be solved as a series of individual uncoupled advection-diffusion equations for each of the velocity components and as an equation for the pressure [5]. As a result of the segregated treatment of the equations however, the solution contains an additional source of temporal error, denoted as the splitting error [5,34]. In addition, by treating the non-linear convection term implicitly (a fully implicit discretization), an iterative method is required to resolve the nonlinearities. Therefore, the solution contains three temporal error components: time integration error (discretization of the time derivative), splitting error, and non-linear iterative error [3]. Here, the solution field at each (implicit) stage of the ESDIRK schemes is computed using an iterated PISO algorithm [42,44] (no under-relaxation is considered in this thesis). The PISO
method is used to increase the rate of convergence of the iterations (and accordingly
the rate at which the splitting error and the non-linear iterative error reduce) [44].

Within an implicit stage \( k \) of the ESDIRK schemes, and at each iteration \( j \) of
the iterated PISO algorithm, the following steps are performed:

1. Solve the discretized momentum equation (predictor step). To proceed with
the computations at each iteration \( j \), previous iteration values are used for the
variables which need to be guessed (i.e. pressure, volumetric flow rate, etc).

\[
\tilde{a}_p U^*_P - \sum_{N=\text{a}(P)} a_N U^*_N = \frac{1}{\Delta t a_{kk}} U^*_P - (\nabla p^{j-1})_P + r_P + \frac{1}{a_{kk}} \sum_{i=1}^{k-1} a_{ki} F^{(i)}_P, \quad (7.24)
\]

2. Calculate volumetric flow rates (right hand side of the pressure equation (7.21)):

\[
\phi^*_f = \left( \frac{1}{\tilde{a}_f} U^n_f + \frac{H_f}{\tilde{a}_f} + \frac{1}{a_{kk}} \sum_{i=1}^{k-1} a_{ki} F^{(i)}_f \right) \cdot n_f S_f, \quad (7.25)
\]

where \( H_f \) and \( \tilde{a}_f \) are computed according to (7.17) and (7.18) respectively.

3. Solve the equation for pressure.

\[
\sum_f \left( \frac{1}{\tilde{a}_f} (\nabla p^j)_f \right) \cdot n_f S_f = \sum_f \phi^*_f. \quad (7.26)
\]

4. Correct the volumetric flow rate, the convective and cell-center velocity fields.

\[
U^j_f = \frac{1}{\Delta t a_{kk}} U^n_f + \frac{H_f}{\tilde{a}_f} - (\nabla p^j)_f + \frac{1}{a_{kk}} \sum_{i=1}^{k-1} a_{ki} F^{(i)}_f, \quad (7.27)
\]

\[
\phi^j_f = U^j_f \cdot n_f S_f, \quad (7.28)
\]

\[
U^j_P = \frac{1}{\Delta t a_{kk}} U^n_P + \frac{H_P}{\tilde{a}_P} - (\nabla p^j)_P + \frac{1}{a_{kk}} \sum_{i=1}^{k-1} a_{ki} F^{(i)}_P. \quad (7.29)
\]

The PISO loop consists of performing steps 2–4 (at least) twice. At the beginning
of each PISO loop, \( H_P(U) \) (which is used in the evaluation of \( H_f(U) \), (7.17))
is computed based on the current value of \( U_P \). Furthermore, within each outer
iteration \( j \), the coefficients of the discretization matrices (\( \tilde{a}_P \), \( a_N \), and accordingly
\( \tilde{a}_f \)) remain constant, but change from one outer iteration to another.

It is pointed out in Issa [15] that each additional PISO-iteration increases the
order of accuracy of the splitting error by one. However, noting that in each outer
iteration \( j \), solving the elliptic pressure equation is typically the most time consuming
part, performing more PISO-loops to lower the splitting error does not seem to offer
significant advantage over performing a complete outer iteration.

After performing sufficient iterations to resolve the nonlinearities in the momentum
equation and the coupling between the equations to a specified tolerance, the
cell-center and face residual vectors are computed using (7.8) and (7.20) respectively.
7.6 Numerical examples and discussion

Three test cases are considered in this section, in order to demonstrate the temporal order preservation of the presented algorithm.

7.6.1 Lid driven cavity flow

The first test case is a two-dimensional lid driven cavity flow with \( Re = \frac{LU_{lid}}{\nu} = 10 \) \((U_{lid}: \text{lid speed, } L: \text{height of the cavity, } \nu: \text{fluid kinematic viscosity})\). The domain is a unit square surrounded by solid walls. The top wall is sliding to the right with a velocity of magnitude \( U_{lid} = 1 \). A uniform grid of \( 50 \times 50 \) has been used. The convective and diffusive terms are discretized using centered schemes. The no slip boundary condition is imposed for the velocity at the walls, and zero gradient for the pressure. At each stage the linear system for each flow variable is solved to a tolerance of \( \varepsilon_{\text{solver}} < 10^{-15} \). In addition, the solution algorithm is iterated to a strict tolerance of \( \varepsilon_{\text{iter}} < 10^{-11} \) to eliminate iteration error (splitting error and non-linear iterative error) as a contaminating variable in the study. \( \varepsilon_{\text{iter}} \) is the \( L_2 \) norm of the magnitude of the residual vector \( \mathbf{R} \) of the fully-discretized momentum equation. The residual vector \( \mathbf{R}_j \) at each iteration has been computed using,

\[
\mathbf{R}_j^p = -\frac{U_j^p - U_n^p}{\Delta t a_{kk}} + \mathbf{F}_j^p + \frac{1}{a_{kk}} \sum_{i=1}^{k-1} a_{ki} \mathbf{F}_p^{(i)}. \quad (7.30)
\]

Furthermore, at each iteration \( j \), two PISO iterations are used.

A few definitions which will be used throughout this section are given here. The temporally exact solution \( U_{\text{exact}} \) is defined as one acquired by solving the problem using a fine time-step size. The time integration error \( \epsilon_t \) is defined as the difference between the temporally exact solution and the solution obtained using a coarse time-step size relative to the temporally exact solution \( \epsilon_t = U_{\text{exact}} - U \) (assuming that the iteration error is negligible).

The temporal accuracy of the algorithm was investigated by considering the cavity flow start-up process. The fluid is initially at rest and computations are carried out to \( t_{\text{final}} = 0.05 \). The (time integration) error is evaluated by comparing the results at \( t_{\text{final}} \). The temporally exact solution is obtained using the fifth order ESDIRK (ESDIRK5) with time step-size of \( \Delta t_{\text{fine}} = 1 \times 10^{-4} \). The error in the cell-center velocity and pressure are shown as a function of time step size, in respectively Fig. 7.2a, and Fig. 7.2b. The maximum Courant number at \( t_{\text{final}} \) using ESDIRK-5 and \( \Delta t = 0.01 \) was \( Co = 0.45 \).

As the results demonstrate, the design orders of the 3\(^{rd}\)-5\(^{th}\) order ESDIRK schemes (denoted in the figures by ESDIRK3 to ESDIRK5) are clearly observable in both the velocity and pressure fields. Furthermore, the pressure appears to be more sensitive (in comparison to the velocity field) to the imposed iterative tolerance \( (\epsilon_{\text{iter}} < 10^{-11}) \) and the accuracy of the solution does not increase by reducing the time-step size once the error in the solution reaches the tolerance.
Since $\frac{1}{a_k} \sum_{i=1}^{k-1} a_k \mathbf{F}^{(i)}_p$ in (7.15) does not explicitly depend on $\Delta t$, it might appear that it is possible to include it in $\mathbf{H}_p$ (i.e. $\mathbf{F}_f = [\mathbf{F}_p]_f$); hence in evaluating $U_f$, there is no need for defining an additional variable $\mathbf{F}_f$. Temporal order analysis was also carried out for this solution algorithm. For each ESDIRK scheme, its solution at $t_{final}$ obtained with a time step-size of $\Delta t_{fine} = 1 \times 10^{-5}$ was used as the temporally exact solution. As Fig. 7.3 demonstrates, by using this algorithm the solution accuracy reduces to first order in the asymptotic range.

Figure 7.2: Error as a function of $\Delta t$ in (a) Cell-center velocity field magnitude, and (b) pressure field.

Figure 7.3: Error as a function of $\Delta t$ in (a) Cell-center velocity field magnitude, and (b) pressure field, for the algorithm where sum of the previously evaluated cell center residual vectors $\mathbf{F}_p$ is included in $\mathbf{H}_p$. 
7.6.2 Lid driven cavity flow-Unstructured Grid

We continue to look at the lid driven cavity test case. The Reynolds number is increased to \( Re = \frac{UL}{\nu} = 100 \). This time an unstructured triangular mesh with 3448 vertices and 6678 cells was generated and is shown in Fig. 7.4. In the momentum and pressure equations, the discretization of the face-normal gradient of respectively the velocity components and the pressure includes two terms (see [17, 42] for more details): an orthogonal contribution which is treated implicitly, and a non-orthogonal correction which is treated explicit (lags behind by one iteration). In correcting the face velocity vector \( U_f^j \), (7.27), the face normal pressure gradient is evaluated by computing the orthogonal term using the updated pressure field \( (p^j) \) and the non-orthogonal term using the pressure field at the previous iteration \( (p^{j-1}) \); this is necessary to ensure mass conservation.

![Unstructured mesh for flow in cavity.](image)

At each stage the following algorithm tolerances are imposed: \( \varepsilon_{\text{solver}} < 10^{-15} \), \( \varepsilon_{\text{iter}} < 10^{-12} \). Again 2-PISO iterations are performed in each outer iteration \( (j) \). Similar to the previous test case, the temporal accuracy of the algorithm is investigated by considering the cavity flow start-up process. The fluid is initially at rest and computations are carried out to \( t_{\text{final}} = 0.5 \). The temporally exact solution was obtained using the fifth order ESDIRK (ESDIRK5) with a time step-size of \( \Delta t_{\text{fine}} = 10^{-4} \). The (time integration) error in the cell-center velocity and pressure are shown as a function of time step size, in respectively Fig. 7.5a, and Fig. 7.5b. The maximum Courant number at \( t_{\text{final}} \) using ESDIRK-5 with \( \Delta t = 0.05 \) is \( Co = 5.0 \).

As the results demonstrate, the design orders of the 3rd,5th order ESDIRK schemes are preserved on the unstructured mesh in both the velocity and pressure fields.
The next test case is an oscillatory lid driven cavity, where a sinusoidal forcing function is imposed on the top wall,

\[ U_{lid} = \sin(\pi t), \]  

(7.31)

where \( \pi \) is the frequency of the oscillation, and is related to the period of the oscillations (\( T \)) by \( T = \frac{2\pi}{\pi} \). This test case has been studied for example in [16,29,39]. Here, simulations are performed for \( Re = 400 \) and frequency of \( \pi = 0.5\pi \). A uniform grid of 129 \( \times \) 129 has been used.

Fig. 7.6 shows the time evolution, during a few cycles, of the \( x \)-component of the velocity field at the midplane \( x = 0.5 \) for locations \( y = 0.25, y = 0.5, \) and \( y = 0.75 \). After an initial transient phase (the fluid is initially at rest), the oscillatory flow reaches a periodic state. The flow is periodic at all locations and amplitude of the oscillation decreases away from the oscillatory wall. Furthermore, there is a phase shift between the lid motion and flow in the cavity, and among different locations in the flow.

The temporal accuracy of the algorithm is investigated by comparing the results during one cycle in the periodic state. At each stage the following algorithm tolerances are imposed: \( \epsilon_{sol} < 10^{-15}, \epsilon_{iter} < 10^{-13} \). Again 2-PISO iterations are performed in each outer iteration \((j)\). The temporally exact solution is obtained using ESDIRK-5 scheme with \( \Delta t = T/1024 \). The (time integration) error in the cell-center velocity and pressure are shown as a function of time step size, in respectively Fig. 7.7a, and Fig. 7.7b. The maximum Courant number during the simulation using ESDIRK-5 with \( \Delta t = T/8 \) was \( Co \approx 60 \).

As the results in the figures demonstrate, temporal design order is preserved in all the flow variables.
7.7 Conclusions

The high order ESDIRK schemes have been used for advancing the solution to the unsteady INS in time. The cell-centered collocated finite volume method has been used for spatial discretization. A face velocity interpolation procedure which preserves temporal design order of the multi-stage ESDIRK schemes has been introduced. In addition, the influence of iterative errors on temporal order is minimized by using an iterative time advancing algorithm (iterated-PISO). The results from

Figure 7.6: Time evolution of the x-component of the velocity field during a few cycles in several locations along the midplane \( x = 0.5 \).

Figure 7.7: Error as a function of \( \Delta t \) in (a) Cell-center velocity field magnitude, and (b) pressure field.
solving three numerical examples, demonstrated the temporal order preservation of the algorithm.
Chapter 8

Conclusions and Recommendations

8.1 Conclusions

Conjugate heat transfer (CHT) encountered in many engineering applications is unsteady, and accurate determination of the transients is essential in enhancing efficiency and/or safety of designs. However, time-accurate computations of CHT can be computationally expensive. Furthermore, given the multi-physics nature of many engineering problems, resolution of other coupled phenomena, in addition to CHT, may also be of interest. This thesis aimed at developing flexible and efficient numerical procedures for solving unsteady (transient) conjugate heat transfer. In order to reduce the computational work of solving time-accurate CHT problems, high order implicit schemes (which have the potential to improve computational efficiency relative to the commonly used second order schemes) have been considered for time integration. Furthermore, the partitioned method has been adopted which provides a flexible means of using much of the already existing efficient and highly optimized separate fluid and solid physics solvers. Depending on the strength of the thermal interaction between the subdomains, it is in general computationally more efficient to select either a loosely-coupled or strongly-coupled algorithm. The ratio of the thermal effusivities of the coupled domains denoted by $\sigma$ is used as a measure of the strength of the thermal interaction: when $\sigma \ll 1$, the strength of the interaction is weak, and as $\sigma \to 1$ the strength of the interaction increases.

ESDIRK schemes and a strongly coupled solution algorithm

For strongly coupled problems, a time-accurate strongly-coupled solution algorithm has been presented where high order L-stable explicit first stage singly diagonally implicit Runge-Kutta (ESDIRK) schemes are used to advance the solution in time within each subdomain. Interface iterations (subiterations) are performed (at each stage) to retain stability and/or to increase the accuracy of the partitioned solution.
For Dirichlet-Neumann conditions at the interface, the stability and rate of convergence of performing (Gauss-Seidel) subiterations at each stage of the ESDIRK schemes were analyzed analytically. The following conclusions were obtained based on the analysis:

- For stability of the partitioned algorithm, the domain with the higher effusivity is assigned the Neumann condition and the one with the lower effusivity the Dirichlet condition.

- The interface iterations converge with a rate approximately given by $\sigma$. For cases where $\sigma \ll 1$, subiterations will converge rapidly. However, as $\sigma \to 1$, the convergence rate of the iterations decreases.

- For strongly coupled problems, more robust and efficient subiteration methods such as the Aitken under-relaxation should be used to increase the rate of convergence of the iterations.

**IMEX schemes and a loosely-coupled solution algorithm**

For weakly coupled problems $\sigma \ll 1$, a loosely-coupled solution algorithm is presented in which a family of high order implicit-explicit (IMEX) Runge-Kutta schemes are used for time integration. The IMEX schemes consist of the ESDIRK schemes which are used for advancing the solution in time within each separate fluid and solid subdomain and equal order and number of stages explicit Runge-Kutta (ERK) schemes for explicit integration of part of the coupling terms. Dirichlet-Neumann interface conditions are used for spatial coupling between the subdomains. Interface boundary conditions are imposed according to the criterion obtained for the strongly coupled approach.

Given the multiple stages, applying analytical methods to study the numerical properties of the loosely coupled IMEX schemes is not straightforward. However, because of similarities between the second stage of the loosely-coupled IMEX and the predictor-corrector Crank-Nicolson scheme, analytical accuracy and stability analysis is performed for the latter scheme. The following conclusions were obtained based on the analyses:

- Based on the accuracy analysis, the design order of the time integration scheme is preserved by following a predictor (implicit)-corrector (explicit) approach at each time-step. Therefore, the need to subiterate at each time-step is avoided.

- The analytical stability analysis shows that by using the Crank-Nicolson scheme for time integration, the partitioned algorithm is unstable for large Fourier numbers, unlike the monolithic approach. This is also in contrast to the unconditional stability of the partitioned algorithm with Backward Euler for time integration.
For stable computations using the predictor-corrector Crank-Nicolson scheme, the stability criterion $\sigma \sqrt{d_1 d_2} < \gamma$ needs be satisfied. $d_m$ with $m = 1, 2$ is the Fourier number of each subdomain, and $\gamma$ is equal 1 for the vertex-based discretization and 2/3 for the cell-center discretization with linear extrapolation of the interface temperature.

Next, the accuracy and stability of the loosely-coupled IMEX algorithm were investigated numerically. The following conclusions were drawn:

- The loosely-coupled algorithm preserves the temporal order of the IMEX schemes without subiterating at each stage.
- Similar to the predictor-corrector Crank-Nicolson, the product $\sigma \sqrt{d_1 d_2}$ has an influential effect on the stability of the algorithm.
- The variable $\sigma$, can be used to identify a class of problems which the loosely coupled IMEX schemes are appropriate to apply to. For weakly coupled problems ($\sigma \ll 1$), the algorithm remains stable to large Fourier numbers $d_m$, indicating that time-step size is restricted by accuracy rather than stability. However, as $\sigma$ approaches unity, the stability and accuracy of the schemes reduce.
- The IMEX schemes have better stability properties compared to the predictor-corrector Crank-Nicolson scheme.

**Computational efficiency analysis**

The computational work of the high order time integration schemes relative to second order schemes was another topic which was investigated in the thesis. For both the loosely and strongly coupled solution algorithms, by respectively considering a weakly coupled and a strongly coupled CHT test-case, the work-precision character of the high order time integration schemes and the commonly used second order schemes were compared over a range of accuracy requirements. For the weakly coupled problem, the high order IMEX schemes (in particular the fourth and fifth order) were observed to be 1.5 times more efficient than Crank-Nicolson and 2.7 times more efficient than BDF2 for time-accurate solutions. In addition, the loosely-coupled IMEX schemes were observed to be as efficient as the monolithic ESDIRK schemes. For the strongly coupled problem, by using the strongly-coupled ESDIRK schemes gain in computational efficiency relative to the Crank-Nicolson was observed (for time-accurate solutions, a factor of 1.8 using ESDIRK4). Furthermore, for both the weakly and strongly coupled CHT test-cases, the computational gain from using the high order schemes increased (relative to the work of the second order schemes) as smaller tolerances were sought.

In addition, the efficiency investigation demonstrated that when the solution varies smoothly with time, the (A-stable) Crank-Nicolson scheme can be computationally competitive (for a reasonable range of temporal accuracy) with the high
order ESDIRK schemes (particularly ESDIRK3).

**ESDIRK schemes and collocated FV discretization of the INS**

For the (loosely and/or strongly coupled) partitioned algorithms to preserve the temporal design order, it is necessary for the separate physics solvers to have the correct order behavior for the *uncoupled simulations*. In this thesis, application of high order ESDIRK schemes to (cell-centered) collocated finite volume discretization of unsteady incompressible flows was considered. In particular, a face-velocity interpolation procedure which preserves the temporal design order of the multi-stage ESDIRK schemes has been introduced. In addition, the influence of iterative errors on temporal order is minimized by using an iterative time advancing algorithm. The results from solving numerical examples, demonstrated the temporal order preservation of the algorithm.

### 8.2 Recommendations

In this section, we briefly describe some additional issues on increasing computational efficiency, and some possible directions for further research based on the current work.

In the present study, a fixed time step was used for all simulations. For a fixed temporal accuracy, however, the time step usually varies during a typical simulation [1]. Therefore, a fixed time step may not be the optimal choice. The Runge-Kutta schemes include embedded schemes which allow for the use of automatic error-based time-step controllers; for examples, see [2] (a CHT problem), [41] (incompressible flow) and [1,3,21,23] (CDR and compressible flow problems using the Runge-Kutta schemes of [23] considered in this paper).

One of the factors which will reduce the efficiency of strongly coupled algorithms is solving the interface (or fixed-point) iterations at each stage (step) to inappropriate subiteration tolerance levels. Once the partitioning error is below the time integration error, performing additional subiterations does not increase the solution accuracy, but does increase the computational cost. One the other hand, if sufficient subiterations are not performed, the partitioned solution is dominated by the partitioning error which will result in the deterioration of the solution accuracy and/or instability. Within each physics solver, an analogous situation also holds between the iteration error (such as splitting error and non-linear iterative error) and the time integration error. An additional benefit of the error estimate is providing a termination strategy for the interface iterations as well as the nonlinear iterations (of the physics solvers). For details and examples refer to [1–3].

For strongly coupled problems, the Dirichlet-Neumann interface conditions have a slow convergence rate when Block Gauss-Seidel iteration are performed. One approach to increase the convergence rate is to employ more robust iterative methods.
The Aitken under-relaxation for example was used in Chapter 6 to demonstrate the approach. Increased convergence rate may also be achieved by using other transmission conditions at the interface. In [14], the convergence rate of performing Block Gauss-Seidel iteration using mixed conditions at the interface is analyzed. For strongly coupled problems, faster convergence rates compared to the Dirichlet-Neumann interface conditions were observed.

Applying the mixed conditions at the interface in loosely-coupled algorithms is another possible direction. It would be interesting to investigate whether the mixed interface conditions will improve the temporal accuracy and stability of the loosely coupled algorithm compared Dirichlet-Neumann as the strength of thermal interaction is increased.

Another interesting direction for this work is to add radiation effects to the coupled problem. This will result in the addition of a non-linear term in interface flux equation. There are already works in the literature on this topic such as [45, 46] where, for steady-state computations, stability of subiteration techniques for partitioned simulation of the coupled problem have been studied. For transient cases using high order implicit schemes for time integration, such as the ESDIRK and possibly the IMEX, stability and temporal order preservation of the partitioned algorithms are issues that need to be investigated.
Appendix A

Stability analysis without update of interface conditions

In this appendix, we consider the stability of the loosely-coupled partitioned algorithm given in Algorithm 2 (the $\theta$ scheme for time integration, and integrating $\Omega_1$ first, BGS-12). As the algorithm demonstrates, the interface conditions are not updated at the end of each time step. As a result, in the next time step, in computing the solution to $T_{n+1}^{1.0}$ (4.15), the interface flux $q_{1,0}^n$ in $F_1^n$ is equal to $q_{2,0}^{n-1}$:

$$q_{1,0}^n = q_{1,0}^{n-1} = -\frac{k_2}{\Delta x_2}(T_{2,0}^{n-1} - T_{2,0}^{n-1}).$$ (A.1)

If the interface equations would have been updated at the end of each time-step, then $q_{1,0}^n$ was given by (4.37). Furthermore, the interface heat flux at $t^{n+1}$, $q_{1,0}^{n+1}$, is predicted using the previous time step solution of $q_{2,0}$, as (4.36) shows. In addition, noting that BGS-12 is used to solve the coupled problem, $T_{2,0}^{n+1} = T_{1,0}^{n+1}$, $T_{2,0}^n = T_{1,0}^n$, and $T_{2,0}^{n-1} = T_{1,0}^{n-1}$.

The resultant system of equations for this loosely-coupled partitioned algorithm where $\Omega_1$ is integrated first (BGS-12) is given by:

$$T_{1,j}^{n+1} = T_{1,j}^n + \theta d_1(T_{1,j-1} - 2T_{1,j} + T_{1,j+1})^{n+1}$$
$$+ (1 - \theta)d_1(T_{1,j-1} - 2T_{1,j} + T_{1,j+1})^n \quad j < 0,$$

$$T_{1,0}^{n+1} = T_{1,0}^n - 2\theta d_1(T_{1,0} - T_{1,-1})^{n+1} - 2(1 - \theta)d_1(T_{1,0} - T_{1,-1})^n$$
$$+ 2\theta rd_2(T_{2,1} - T_{2,0})^{n+1} + 2(1 - \theta)rd_2(T_{2,1} - T_{2,0})^n,$$

$$T_{2,j}^{n+1} = T_{2,j}^n + \theta d_2(T_{2,j-1} - 2T_{2,j} + T_{2,j+1})^{n+1}$$
$$+ (1 - \theta)d_2(T_{2,j-1} - 2T_{2,j} + T_{2,j+1})^n \quad j > 0,$$

$$T_{2,0}^{n+1} = T_{1,0}^{n+1},$$

$$T_{2,0}^n = T_{1,0}^n,$$

$$T_{2,0}^{n-1} = T_{1,0}^{n-1}.$$ (A.2)
Following Giles [11], the stability of the loosely coupled algorithm is analyzed by expressing the form of the solution using normal modes. For this partitioned algorithm, the form of the normal mode solution is given by (4.42). The three last equations in (A.2) are satisfied as a result of the selected normal modes. The other equations in (A.2) require that the variables \(z\), \(\kappa_1\) and \(\kappa_2\) satisfy the equations:

\[
\begin{align*}
1 &= z^{-1} + d_1(\kappa_1 - 2 + \kappa_1^{-1})(\theta + (1 - \theta)z^{-1}) , \\
1 &= z^{-1} + 2d_1(-1 + \kappa_1^{-1})(\theta + z^{-1}(1 - \theta)) + 2rd_2z^{-1}(\kappa_2 - 1)(\theta + z^{-1}(1 - \theta)) , \\
1 &= z^{-1} + d_2(\kappa_2 - 2 + \kappa_2^{-1})(\theta + (1 - \theta)z^{-1}) .
\end{align*}
\] (A.3)

Solving the first and last equations for \(\kappa_1^{-1}\) and \(\kappa_2\) we obtain (4.44). To satisfy the farfield boundary conditions, we must have \(|\kappa_1^{-1}| < 1\) and \(|\kappa_2| < 1\). Thus, for the case of real and positive arguments within the square-roots, this means that the negative roots must be selected. Substituting the two into the second equation in (A.3), we obtain the equation for the amplification factor, i.e. \(z\):

\[
\sqrt{1 + \frac{4d_1(\theta(1 - z^{-1}) + z^{-1})}{1 - z^{-1}}} + rz^{-1} \left[ \sqrt{1 + \frac{4d_2(\theta(1 - z^{-1}) + z^{-1})}{1 - z^{-1}}} - 1 \right] = 0. \tag{A.4}
\]

Since obtaining a closed form solution to \(z\) is not trivial, usually asymptotic solutions are considered under certain assumptions.

For case of \(d_m \gg 1\), (A.4) reduces to:

\[
\sqrt{\frac{d_1}{d_1}} + rz^{-1} \sqrt{\frac{d_2}{d_2}} \approx 0, \tag{A.5}
\]

with the asymptotic solution given by,

\[
z \approx - \sqrt{\frac{d_2}{d_1}} r . \tag{A.6}
\]

In order to have a stable solution \(|z| < 1\), the stability criterion is given by:

\[
|\sqrt{\frac{d_2}{d_1}} r | < 1. \tag{A.7}
\]

Substituting for \(d_1\), \(d_2\), and \(r\) their corresponding equivalence into (A.7), yields (3.2). The stability criterion is independent of the value of \(\theta\) and the scheme should remain stable for large \(d_m\) numbers by the correct assignment of the interface conditions.
Appendix B

Alternative form of system of equations at each stage of the loosely-coupled algorithm

In this appendix, for the one dimensional model problem described in section 2.2, the parameters that may influence the stability of the loosely-coupled algorithm presented in section 5.1 are identified. To simplify the analysis typically a vertex based rather than cell-centered spatial discretization is preferred (see section 4.1 for details). By applying the IMEX schemes to the semi-discrete form of the problem, the following system of equations at each implicit stage of the loosely-coupled algorithm is obtained (assuming that $\Omega_1$ is integrated first (BGS-12)):

\begin{align*}
T^{(k)}_{1,j} &= T^n_{1,j} + a^{I}_{kk}d_1(T_{1,j-1} - 2T_{1,j} + T_{1,j+1})^{(k)}
+ \sum_{i=1}^{k-1} a^{I}_{ki}d_1(T_{1,j-1} - 2T_{1,j} + T_{1,j+1})^{(i)}, \quad j < 0, \quad (B.1) \\
T^{(k)}_{1,0} &= T^n_{1,0} - 2a^{I}_{kk}d_1(T_{1,0} - T_{1,-1})^{(k)} - \sum_{i=1}^{k-1} 2a^{I}_{ki}d_1(T_{1,0} - T_{1,-1})^{(i)}
+ 2 \sum_{i=1}^{k-1} a^{E}_{ki}\sqrt{d_1d_2}(T_{2,1} - T_{2,0})^{(i)}, \quad (B.2) \\
T^{(k)}_{2,j} &= T^n_{2,j} + a^{I}_{kk}d_2(T_{2,j-1} - 2T_{2,j} + T_{2,j+1})^{(k)}
+ \sum_{i=1}^{k-1} a^{I}_{ki}d_2(T_{2,j-1} - 2T_{2,j} + T_{2,j+1})^{(i)}, \quad j > 0 \quad (B.3) \\
T^{(i)}_{2,0} &= T^{(i)}_{1,0} \quad i = 1, \ldots, k \quad (B.4)
\end{align*}
Bibliography


List of Publications

Journal articles


Conference proceedings


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Curriculum Vitae

11/9/1984 Born in Tehran, Iran.

Dec 2008 – Sept 2013
PhD researcher at Aerospace Engineering Department of Delft University of Technology (TU Delft).
Under supervision of: Prof. dr. ir. drs. H. Bijl and Dr. ir. A.H. van Zuijlen.

June 2008 Master of Engineering at Mechanical Engineering Department of The City College of the City University of New York.
Under supervision of: Prof. Y. Andreopoulos.

June 2006 Bachelor of Engineering at Mechanical Engineering Department of The City College of the City University of New York.
Errata

Page 54 equation (6.6), replace $(\alpha_m \nabla^2 \vartheta_m + f(x, t))^i)$ with $(\alpha_m \nabla^2 \vartheta_m^i(x) + f_m(x, t^{(i)}))$.

Page 55 equation (6.12), replace $f^{(k)}(x)$ with $f_m(x, t^{(k)})$, and replace $(\alpha_m \nabla^2 \vartheta_m(x) + f(x, t))^{(i)}$ with $(\alpha_m \nabla^2 \vartheta_m^i(x) + f_m(x, t^{(i)}))$.

Page 73, last paragraph, replace subscript $i$ with $k$ in $\frac{1}{d_k}$: $\frac{1}{a_k}$.

Page 74 equations 7.15 and 7.16, move superscript $(k)$ outside parenthesis in $(\nabla p^{(k)})$: $(\nabla p)^{(k)}_P$ and $(\nabla p)^{(k)}_f$.

Page 75 equations 7.21, add superscript $(k)$ to $(\nabla p)_f$ and $H_f$: $(\nabla p)^{(k)}_f$ and $H^{(k)}_f$.

Page 76, 3rd line of paragraph after equation (7.29), replace “outer iteration $j$” with “inner (PISO) iteration”.

Page 78, in caption of Fig. 7.2, add $\delta_\ell = |max(\ell) - min(\ell)|$ (with $\ell$ representing $U_{magExact}$ or $P_{Exact}$).

Page 79, first paragraph, add the following sentence at end of line 3: “Linear interpolation is used for discretizing the convective terms”.

Page 80, end of first paragraph, add the following sentence: “The convective and diffusive terms are discretized using second order centered schemes.”.