MY PRELIM

by

Lewis John Lloyd

A preliminary report submitted in partial fulfillment of the requirements for the degree of

Doctor of Philosophy

(Engineering Physics)

at the

UNIVERSITY OF WISCONSIN-MADISON

Acknowledgments

DOE and MUSC encourage fellows to publish reports and articles in scientific and engineering journals. The fellow must submit any articles, reports, or thesis to MUSC prior to submission for publication. All publications will show the joint affiliation of the fellow with the university and, if appropriate, with the laboratory in which the research was conducted, and should acknowledge fellowship support.

Fellowship support should be acknowledged in the following manner:

This research was performed under appointment to the Rickover Fellowship Program in Nuclear Engineering sponsored by Naval Reactors Division of the U.S. Department of Energy.

Table Of Contents

		Pag	je
Li	st Of	Tables	V
Li	st Of	Figures	v
Li	st Of	Algorithms	۷i
No	meno	elature	ii
Al	strac	t vi	ii
1	Intr	roduction	1
	1.1 1.2		1
2	Flui	id Mechanics	3
	2.1	Two Phase Flow	3
3	Ma	thematical Formulation	4
	3.1	3.1.1 Continuity Equations	5 5 7
	3.2	Discrete Hydrodynamic Equations	8 9 2
	3.3 3.4	Structural Thermal Energy Equations	3
	3.5		3
4	Jac	,	4
	4.1 4.2	Newton's Method	4 6 6

Appendix	Apı	pendix
----------	-----	--------

	I	Page
4.2.2	Globalization Strategies	19
APPENDICES		
Appendix A:	: Model stuff	20
Appendix B:	: Model stuff	26
Appendix C:	: Model stuff	32

List Of Tables

Table Page

List Of Figures

Figure Page

List Of Algorithms

Algorithm Page
4.14 Insient Loop14 4.02 lifted Newton's Method - Frozen Jacobian15 4.03 ton's Method17

Nomenclature

$ ho_v$	Gas Density
$ ho_l$	Liquid Density
α_{st}	Steam Volume Fraction
α_l	Continuous Liquid Volume Fraction
α_e	Entrained Liquid Volume Fraction
C_1	Constant 1
V	Voltage
\$	US Dollars

Abstract

First paragraph

Second paragraph

Third paragraph

Chapter 1

Introduction

1.1 Motivation

Of primary use in the field of nuclear reactor safety analysis is simulation. The ability to predict the behaviour of reactors during off-normal events is the key to the licensing and the operation of nuclear power plants. Within the United States, this simulation capacity is provided by a relatively small number of main stream software suites, among which are the RELAP variants, COBRA variants, and MELCOR. While each of these software products varies in their models and implementations, the underlying numeric techniques and capabilities are similar. Traditionally, these system codes utilize a semi-implicit discritization scheme. In order to solve the resulting system of equations, the most common methodology is to take a single networ step. The underlying numeric methods are first order methods.

The ability to use higher order methods is important. Since the development of the semiimplicit method, whose form was motivated by the limited computer resources available at the time, there have been great advances in both the methodology used to solve linear algebra problems and computer capabilities.

1.2 Objectives

The objective of this dissertation is the design, implementation, and evaluation of a practical non-linear solution framework for reactor safety systems codes. Specifically, an efficient and reliable solution methodology to the two-phase, three-field, fluid-dynamics and the solid-structure heat transfer system of coupled non-linear partial differential equations is sought. The specific

methodology should be capable of obtaining a consistent solution to the system of PDEs while also possessing.

Chapter 2

Fluid Mechanics

Of primary concern in reactor safety analysis is thermal-hydraulic behaviour of the nuclear core during off-normal conditions. In order to evaluate

2.1 Two Phase Flow

The physical behaviour of fluids within COBRA are represented by a set of differential equations. These governing equations are a collection of balance laws. Balance laws are statements of conservation that include external sources and sinks. The physical quantities being tracked by COBRA are mass, momentum, and energy. Since COBRA models two phase behaviour, the

Chapter 3

Mathematical Formulation

As mentioned earlier, most reactor safety-analysis codes depend upon three discrete sets of physics. These include, but are not necessarily limited to, two-phase hydrodynamics, heat-transfer between the fluid and a solid structure, and a nuclear power source. The different physical phenomena are represented by a system of PDEs and ODEs that constitute a set of balance laws for mass, momentum, and energy. This system encompasses different scales in both space and time.

3.1 Hydrodynamic Conservation Equations

Conserved Variables

Independent Variables

$$\underline{\mathbf{q}} = \begin{bmatrix}
\alpha \rho_{g} \\
\alpha (\rho_{v} + \rho_{g}) \\
(1 - \alpha) \rho_{l} \\
\alpha_{e} \rho_{l} \\
(1 - \alpha) \rho_{l} \underline{\mathbf{U}}_{v} \\
(1 - \alpha) \rho_{l} \underline{\mathbf{U}}_{l} \\
\alpha_{e} \rho_{l} \underline{\mathbf{U}}_{e} \\
\alpha (\rho_{v} + \rho_{g} H_{g}) \\
(1 - \alpha) \rho_{l} H_{l}
\end{bmatrix}$$

$$(3.1) \qquad \underline{\mathbf{x}} = \begin{bmatrix}
\alpha \\
\alpha P \\
\alpha P_{g} \\
\alpha (\rho_{v} + \rho_{g}) \underline{\mathbf{U}}_{v} \\
(1 - \alpha) \rho_{l} \underline{\mathbf{U}}_{l} \\
\alpha_{e} \rho_{l} \underline{\mathbf{U}}_{e} \\
\alpha H_{v} \\
(1 - \alpha) H_{l}
\end{bmatrix}$$
Note that $\mathbf{q} = f(\underline{\mathbf{x}})$.

3.1.1 Continuity Equations

3.1.1.1 Mass

$$\underline{\mathbf{x}} = \begin{bmatrix} \alpha \\ \alpha_e \\ P \\ \alpha P_g \\ \alpha (\rho_v + \rho_g) \underline{\mathbf{U}}_v \\ (1 - \alpha) \rho_l \underline{\mathbf{U}}_l \\ \alpha_e \rho_l \underline{\mathbf{U}}_e \\ \alpha H_v \\ (1 - \alpha) H_l \end{bmatrix}$$
(3.3)

$$\frac{\partial}{\partial t}\alpha_g \rho_g + \nabla \cdot (\alpha_g \rho_g \underline{\mathbf{U}}_g) = \Gamma''' \tag{3.4}$$

$$\frac{\partial}{\partial t} \alpha_l \rho_l + \nabla \cdot (\alpha_l \rho_l \underline{\mathbf{U}}_l) = -(1 - \eta) \Gamma''' - S'''
\frac{\partial}{\partial t} \alpha_e \rho_l + \nabla \cdot (\alpha_e \rho_l \underline{\mathbf{U}}_e) = -\eta \Gamma''' + S'''$$
(3.5)

$$\frac{\partial}{\partial t} \alpha_e \rho_l + \nabla \cdot (\alpha_e \rho_l \underline{\mathbf{U}}_e) = -\eta \Gamma''' + S'''$$
(3.6)

$$\frac{\partial}{\partial t}\alpha_g \rho_{nc} + \nabla \cdot (\alpha_g \rho_{nc} \underline{\mathbf{U}}_g) = \Gamma''' \tag{3.7}$$

$$(\alpha \rho_{v})^{n+1} + \frac{\Delta t}{V_{c}} \left[\sum_{J} \left[\frac{(\alpha \rho_{v})^{*}}{\langle \alpha \rho_{v} \rangle} \right]^{n} \underline{\dot{\mathbf{M}}}_{v}^{n+1} \cdot \hat{\mathbf{n}} + \sum_{K} \left[\frac{(\alpha \rho_{v})^{*}}{\langle \alpha \rho_{v} \rangle} \right]^{n} \underline{\dot{\mathbf{W}}}_{v}^{n+1} \cdot \hat{\mathbf{n}} \right]$$

$$= (\alpha \rho_{v})^{n} + \frac{\Delta t}{V_{c}} \Gamma^{n+1}$$

$$(3.8)$$

$$(\alpha \rho_{g})^{n+1} + \frac{\Delta t}{V_{c}} \left[\sum_{J} \left[\frac{(\alpha \rho_{g})^{*}}{\langle \alpha \rho_{g} \rangle} \right]^{n} \underline{\dot{\mathbf{M}}}_{v}^{n+1} \cdot \hat{\mathbf{n}} + \sum_{K} \left[\frac{(\alpha \rho_{g})^{*}}{\langle \alpha \rho_{g} \rangle} \right]^{n} \underline{\dot{\mathbf{W}}}_{v}^{n+1} \cdot \hat{\mathbf{n}} \right]$$

$$= (\alpha \rho_{g})^{n}$$

$$(3.9)$$

$$(\alpha_{l}\rho_{l})^{n+1} + \frac{\Delta t}{V_{c}} \left[\sum_{J} \left[\frac{(\alpha_{l}\rho_{l})^{*}}{\langle \alpha_{l}\rho_{l} \rangle} \right]^{n} \underline{\dot{\mathbf{M}}}_{l}^{n+1} \cdot \hat{\mathbf{n}} + \sum_{K} \left[\frac{(\alpha_{l}\rho_{l})^{*}}{\langle \alpha_{l}\rho_{l} \rangle} \right]^{n} \underline{\dot{\mathbf{W}}}_{l}^{n+1} \cdot \hat{\mathbf{n}} \right]$$

$$= (\alpha_{l}\rho_{l})^{n} + \frac{\Delta t}{V_{c}} \left(S_{D}^{n+1} - (1 - \eta^{n}) \Gamma_{l}^{n+1} - S_{E}^{n+1} \right)$$

$$(\alpha_{e}\rho_{l})^{n+1} + \frac{\Delta t}{V_{c}} \left[\sum_{J} \left[\frac{(\alpha_{e}\rho_{l})^{*}}{\langle \alpha_{e}\rho_{l} \rangle} \right]^{n} \underline{\dot{\mathbf{M}}}_{e}^{n+1} \cdot \hat{\mathbf{n}} + \sum_{K} \left[\frac{(\alpha_{e}\rho_{l})^{*}}{\langle \alpha_{e}\rho_{l} \rangle} \right]^{n} \underline{\dot{\mathbf{W}}}_{e}^{n+1} \cdot \hat{\mathbf{n}} \right]$$

$$= (\alpha_{e}\rho_{l})^{n} + \frac{\Delta t}{V_{c}} \left(S_{E}^{n+1} - \eta^{n} \Gamma_{e}^{n+1} - S_{D}^{n+1} \right)$$

$$(3.11)$$

3.1.1.2 Energy

$$\frac{\partial}{\partial t} \left(\alpha_{g} (\rho_{v} h_{v} + \rho_{nc} h_{nc}) \right) + \nabla \cdot \left(\alpha_{g} (\rho_{v} h_{v} + \rho_{nc} h_{nc}) \underline{\mathbf{U}}_{g} \right)
= \Gamma''' h'_{v} + q'''_{i,v} + q'''_{gl} + q'''_{wg} + \alpha_{g} \frac{\partial P}{\partial t}
\frac{\partial}{\partial t} \left((\alpha_{e} + \alpha_{l}) \rho_{l} h_{l} \right) + \nabla \cdot \left(\alpha_{l} \rho_{l} h_{l} \underline{\mathbf{U}}_{l} \right) + \nabla \cdot \left(\alpha_{e} \rho_{l} h_{l} \underline{\mathbf{U}}_{e} \right)
= \Gamma''' h'_{v} + q'''_{i,v} + q'''_{gl} + q'''_{wg} + \alpha_{g} \frac{\partial P}{\partial t}$$
(3.12)

$$(\alpha_{g}(\rho_{v}h_{v} + \rho_{nc}h_{nc}))^{n+1} - \alpha_{g}^{n}P^{n+1} + \frac{\Delta t}{V_{c}} \sum_{J} \left(\frac{(\alpha_{g}(\rho_{v}h_{v} + \rho_{nc}h_{nc}))^{*}}{<\alpha_{g}(\rho_{v}h_{v} + \rho_{nc}h_{nc})>} \right)^{n} \underline{\mathbf{M}}_{v}^{n+1} \cdot \underline{\hat{\mathbf{n}}}$$

$$+ \frac{\Delta t}{V_{c}} \sum_{K} \left(\frac{(\alpha_{g}(\rho_{v}h_{v} + \rho_{nc}h_{nc}))^{*}}{<\alpha_{g}(\rho_{v}h_{v} + \rho_{nc}h_{nc})>} \right)^{n} \underline{\mathbf{W}}_{v}^{n+1} \cdot \underline{\hat{\mathbf{n}}}$$

$$= (\alpha_{g}(\rho_{v}h_{v} + \rho_{nc}h_{nc}))^{n} - \alpha_{g}^{n}P^{n} + \frac{\Delta t}{V_{c}} \left(q_{wg}^{n} + q_{i,v}^{n} + \Gamma^{n}h_{v}^{\prime n} + q_{gl}^{n} \right)$$

$$((\alpha_{e} + \alpha_{l})\rho_{l}h_{l})^{n+1} - (\alpha_{e} + \alpha_{l})^{n}P^{n+1}$$

$$+ \frac{\Delta t}{V_{c}} \sum_{J} \left[\left(\frac{(\alpha_{l}\rho_{l}h_{l})^{*}}{<\alpha_{l}\rho_{l}h_{l}>} \right)^{n} \underline{\mathbf{M}}_{l}^{n+1} \cdot \underline{\hat{\mathbf{n}}} + \left(\frac{(\alpha_{e}\rho_{l}h_{l})^{*}}{<\alpha_{e}\rho_{l}h_{l}>} \right)^{n} \underline{\mathbf{M}}_{e}^{n+1} \cdot \underline{\hat{\mathbf{n}}} \right]$$

$$+ \frac{\Delta t}{V_{c}} \sum_{K} \left[\left(\frac{(\alpha_{l}\rho_{l}h_{l})^{*}}{<\alpha_{l}\rho_{l}h_{l}>} \right)^{n} \underline{\mathbf{W}}_{l}^{n+1} \cdot \underline{\hat{\mathbf{n}}} + \left(\frac{(\alpha_{e}\rho_{l}h_{l})^{*}}{<\alpha_{e}\rho_{l}h_{l}>} \right)^{n} \underline{\mathbf{W}}_{e}^{n+1} \cdot \underline{\hat{\mathbf{n}}} \right]$$

$$= ((\alpha_{e} + \alpha_{l})\rho_{l}h_{l})^{n} - (\alpha_{e} + \alpha_{l})^{n}P^{n} + \frac{\Delta t}{V_{c}} \left(q_{wl}^{n} + q_{i,l}^{n} - \Gamma^{n}h_{l}^{\prime n} - q_{gl}^{n} \right)$$

$$(3.15)$$

3.1.2 Momentum

3.1.2.1 Axial Momentum

$$\frac{\partial}{\partial t} \left(\alpha_{g} (\rho_{v} + \rho_{nc}) \underline{\mathbf{U}}_{g} \right) + \nabla \cdot \left(\alpha_{g} (\rho_{v} + \rho_{nc}) \underline{\mathbf{U}}_{g} \underline{\mathbf{U}}_{g} \right) =
-\alpha_{g} \nabla P + \alpha_{g} (\rho_{v} + \rho_{nc}) \underline{\mathbf{g}}_{g} - \tau'_{wg} - \tau'_{I_{gl}} - \tau'_{I_{ge}} + \Gamma''' \underline{\mathbf{U}}'$$

$$\frac{\partial}{\partial t} \left(\alpha_{l} \rho_{l} \underline{\mathbf{U}}_{l} \right) + \nabla \cdot \left(\alpha_{l} \rho_{l} \underline{\mathbf{U}}_{l} \underline{\mathbf{U}}_{l} \right) =
-\alpha_{l} \nabla P + \alpha_{l} \rho_{l} \underline{\mathbf{g}}_{g} - \tau'_{wl} + \tau'_{I_{gl}} - \left((1 - \eta) \Gamma''' \underline{\mathbf{U}}' \right) - S''' \underline{\mathbf{U}}'$$

$$\frac{\partial}{\partial t} \left(\alpha_{e} \rho_{l} \underline{\mathbf{U}}_{e} \right) + \nabla \cdot \left(\alpha_{e} \rho_{l} \underline{\mathbf{U}}_{e} \underline{\mathbf{U}}_{e} \right) =
-\alpha_{e} \nabla P + \alpha_{e} \rho_{l} \underline{\mathbf{g}}_{g} - \tau'_{wl} + \tau'_{I_{gl}} - \left(\eta \Gamma''' \underline{\mathbf{U}}' \right) + S''' \underline{\mathbf{U}}'$$
(3.18)

$$F_{g}(\underline{\mathbf{x}}^{n+1}) = \underbrace{E_{g}(\underline{\mathbf{x}}^{n})}^{\text{Purely explicit terms}} - A_{mom,j} \Delta z_{j} \left[\alpha_{g}^{n} \frac{P_{J+1}^{n+1} - P_{J}^{n+1}}{\Delta z_{j}} \right]^{\text{Semi-Implicit Drag Terms}}$$

$$- A_{mom,j} \Delta z_{j} \left[\frac{dP}{dz} \Big|_{w,g}^{*} + \frac{dP}{dz} \Big|_{i,lg}^{*} + \frac{dP}{dz} \Big|_{i,eg}^{*} \right]^{\text{Time rate of change}}$$

$$+ \underbrace{Sp_{g,j}^{n+1}}_{p} - \underbrace{\frac{(M_{g,j}^{n+1} - M_{g,j}^{n})}{\Delta t}}_{\Delta t} \Delta z$$

$$= 0$$

3.1.2.2 Transverse Momentum

$$\frac{\partial}{\partial t} \left(\alpha_{g} (\rho_{v} + \rho_{nc}) \underline{\mathbf{V}}_{g} \right) + \nabla \cdot \left(\alpha_{g} (\rho_{v} + \rho_{nc}) \underline{\mathbf{V}}_{g} \underline{\mathbf{V}}_{g} \right) =
-\alpha_{g} \nabla P - \tau'_{wg} - \tau'_{I_{gl}} - \tau'_{I_{ge}} + \Gamma''' \underline{\mathbf{U}}'$$

$$\frac{\partial}{\partial t} \left(\alpha_{l} \rho_{l} \underline{\mathbf{V}}_{l} \right) + \nabla \cdot \left(\alpha_{l} \rho_{l} \underline{\mathbf{V}}_{l} \underline{\mathbf{V}}_{l} \right) =
-\alpha_{l} \nabla P - \tau'_{wl} + \tau'_{I_{gl}} - \left((1 - \eta) \Gamma''' \underline{\mathbf{U}}' \right) - S''' \underline{\mathbf{U}}'$$

$$\frac{\partial}{\partial t} \left(\alpha_{e} \rho_{l} \underline{\mathbf{V}}_{e} \right) + \nabla \cdot \left(\alpha_{e} \rho_{l} \underline{\mathbf{V}}_{e} \underline{\mathbf{V}}_{e} \right) =
-\alpha_{e} \nabla P - \tau'_{wl} + \tau'_{I_{ge}} - \left(\eta \Gamma''' \underline{\mathbf{U}}' \right) + S''' \underline{\mathbf{U}}'$$
(3.22)

3.2 Discrete Hydrodynamic Equations

3.2.1 Axial Momentum

Linearization of the axial momentum equations in COBRA-IE.

$$\underline{\mathbf{x}}_{k} = \begin{bmatrix} \underline{\dot{\mathbf{M}}}_{k} \\ \Delta \mathbf{P}_{k} \end{bmatrix} = \begin{bmatrix} \dot{M}_{l,k} \\ \dot{M}_{g,k} \\ \dot{M}_{e,k} \\ \Delta \mathbf{P}_{k} \end{bmatrix}$$
(3.23)

Note:

$$\underline{\mathbf{L}}(\underline{\mathbf{x}}_{k}) = \underline{\mathbf{L}} \underline{\dot{\mathbf{M}}}_{k} + \underline{\mathbf{b}} \Delta \mathbf{P}_{k}$$

$$\frac{\partial}{\partial \Delta \mathbf{P}_{k}} [\underline{\mathbf{b}} \Delta \mathbf{P}_{k}] = \underline{\mathbf{b}}$$

$$\frac{\partial}{\partial \underline{\mathbf{N}}(\underline{\mathbf{x}}_{k})} = \frac{\partial}{\partial \underline{\dot{\mathbf{M}}}_{k}} = \underline{\underline{\mathbf{N}}(\underline{\dot{\mathbf{M}}}_{k})}$$

$$\underline{\mathbf{J}}_{k}^{*} = \frac{\partial}{\partial \underline{\dot{\mathbf{M}}}_{k}} = \underline{\underline{\mathbf{L}}} + \underline{\underline{\mathbf{N}}(\underline{\dot{\mathbf{M}}}_{k})}$$

$$\underline{\mathbf{J}}_{k} \delta \underline{\mathbf{x}} = \frac{\partial}{\partial \underline{\mathbf{F}}(\underline{\mathbf{x}}_{k})} \delta \underline{\mathbf{x}} = \underline{\underline{\mathbf{J}}}_{k}^{*} \delta(\underline{\dot{\mathbf{M}}}) + \underline{\mathbf{b}} \delta(\Delta \mathbf{P})$$

Current View Point

$$0 = \underline{\mathbf{F}} (\underline{\mathbf{x}}_{k+1})$$

$$0 = \underline{\mathbf{F}} (\underline{\mathbf{x}}_{k+1}) = \underline{\mathbf{E}} + \underline{\mathbf{L}} (\underline{\mathbf{x}}_{k+1}) + \underline{\mathbf{N}} (\underline{\mathbf{x}}_{k+1})$$

$$0 = \underline{\mathbf{E}} + \underline{\mathbf{L}} (\underline{\mathbf{x}}_{k+1}) + \underline{\mathbf{N}} (\underline{\mathbf{x}}_{k+1})$$

$$0 = \underline{\mathbf{E}} + \underline{\underline{\mathbf{L}}} \underline{\dot{\mathbf{M}}}_{k+1} + \underline{\mathbf{b}} \Delta \mathbf{P}_{k+1} + \underline{\mathbf{N}} (\underline{\mathbf{x}}_{k+1})$$

$$0 = \underline{\mathbf{E}} + \underline{\underline{\mathbf{L}}} \underline{\dot{\mathbf{M}}}_{k+1} + \underline{\mathbf{b}} \Delta \mathbf{P}_{k} + \frac{\partial [\underline{\mathbf{b}} \Delta \mathbf{P}_{k+1}]}{\partial \Delta \mathbf{P}_{k+1}} \delta(\Delta \mathbf{P}) + \underline{\mathbf{N}} (\underline{\mathbf{x}}_{k}) + \frac{\partial [\underline{\mathbf{N}} (\underline{\mathbf{x}}_{k+1})]}{\partial \underline{\mathbf{x}}_{k+1}} [\underline{\mathbf{x}}_{k+1} - \underline{\mathbf{x}}_{k}]$$

$$\begin{split} \underline{\underline{L}} \ & \underline{\dot{\mathbf{M}}}_{k+1} + \underline{\underline{\mathbf{N}}}(\underline{\dot{\mathbf{M}}}_k) \ \underline{\dot{\mathbf{M}}}_{k+1} = -\underline{\mathbf{E}} \ -\underline{\mathbf{b}} \ \Delta \mathbf{P}_k - \underline{\mathbf{N}} \left(\underline{\mathbf{x}}_k\right) - \underline{\mathbf{b}} \ \delta(\Delta \mathbf{P}) + \underline{\underline{\mathbf{N}}}(\underline{\dot{\mathbf{M}}}_k) \underline{\dot{\mathbf{M}}}_k \\ & \left[\underline{\underline{\mathbf{L}}} + \underline{\underline{\mathbf{N}}}(\underline{\dot{\mathbf{M}}}_k)\right] \underline{\dot{\mathbf{M}}}_{k+1} = -\left[\underline{\underline{\mathbf{E}}} \ +\underline{\underline{\mathbf{b}}} \ \Delta \mathbf{P}_k + \underline{\mathbf{N}} \left(\underline{\mathbf{x}}_k\right) - \underline{\underline{\mathbf{N}}}(\underline{\dot{\mathbf{M}}}_k) \ \underline{\dot{\mathbf{M}}}_k\right] - \underline{\underline{\mathbf{b}}} \ \delta(\Delta \mathbf{P}) \\ & \underline{\underline{\mathbf{M}}}_{k+1}^* = -\underline{\underline{\mathbf{f}}} \ -\underline{\underline{\mathbf{J}}}_k^{-*} \underline{\underline{\mathbf{f}}} - \underline{\underline{\mathbf{J}}}_k^{-*} \underline{\underline{\mathbf{b}}} \ \delta(\Delta \mathbf{P}) \\ & \underline{\underline{\dot{\mathbf{M}}}}_{k}^{*+1} = -\underline{\underline{\dot{\mathbf{M}}}}_k^{*+1} = -\underline{\underline{\dot{\mathbf{M}}}}_k^{*+1} \underline{\underline{\mathbf{M}}} \underline{\underline{\dot{\mathbf{M}}}}_k \\ & \underline{\underline{\dot{\mathbf{M}}}}_{k+1}^{*+1} = \underline{\underline{\dot{\mathbf{M}}}}_k^{*+1} + \underline{\underline{\dot{\mathbf{M}}}}_k^{*} \underline{\underline{\dot{\mathbf{M}}}}_k \delta(\Delta \mathbf{P}) \end{split}$$

Relation between Newton step and current formulation.

$$\begin{split} \left[\underline{\underline{\mathbf{L}}} + \underline{\underline{\mathbf{N}}}(\underline{\dot{\mathbf{M}}}_{k})\right] \underline{\dot{\mathbf{M}}}_{k+1} &= -\left[\underline{\mathbf{E}} + \underline{\underline{\mathbf{L}}} \, \underline{\dot{\mathbf{M}}}_{k} + \underline{\mathbf{b}} \, \Delta \mathbf{P}_{k} + \underline{\mathbf{N}} \, (\underline{\mathbf{x}}_{k})\right] - \underline{\mathbf{b}} \, \delta(\Delta \mathbf{P}) + \underline{\underline{\mathbf{L}}} \, \underline{\dot{\mathbf{M}}}_{k} + \underline{\underline{\mathbf{N}}}(\underline{\dot{\mathbf{M}}}_{k}) \, \underline{\dot{\mathbf{M}}}_{k} \\ \left[\underline{\underline{\mathbf{L}}} + \underline{\underline{\mathbf{N}}}(\underline{\dot{\mathbf{M}}}_{k})\right] \underline{\dot{\mathbf{M}}}_{k+1} &= -\underline{\mathbf{F}} \, (\underline{\mathbf{x}}_{k}) - \underline{\mathbf{b}} \, \delta(\Delta \mathbf{P}) + \underline{\underline{\mathbf{L}}}_{k}^{*} \, \underline{\dot{\mathbf{M}}}_{k} \\ \underline{\underline{\dot{\mathbf{M}}}}_{k+1} &= -\underline{\mathbf{F}} \, (\underline{\mathbf{x}}_{k}) - \underline{\mathbf{b}} \, \delta(\Delta \mathbf{P}) + \underline{\underline{\mathbf{J}}}_{k}^{*} \, \underline{\dot{\mathbf{M}}}_{k} \\ \underline{\dot{\mathbf{M}}}_{k+1} &= \underline{\underline{\dot{\mathbf{M}}}}_{k}^{*} - \underline{\underline{\mathbf{J}}}_{k}^{-*} \underline{\mathbf{F}} \, (\underline{\mathbf{x}}_{k}) - \underline{\underline{\mathbf{J}}}_{k}^{-1} \underline{\mathbf{b}} \, \delta \mathbf{P} \\ \underline{\dot{\mathbf{M}}}_{k}^{**} &\xrightarrow{\underline{\dot{\mathbf{M}}}_{k}^{**}} + \underline{d} \underline{\underline{\dot{\mathbf{M}}}}_{k}^{*} \delta(\Delta \mathbf{P}) \\ \underline{\dot{\mathbf{M}}}_{k}^{***} &= \underline{\dot{\mathbf{M}}}_{k}^{*************} + \underline{d} \underline{\underline{\dot{\mathbf{M}}}}_{k}^{*} \delta(\Delta \mathbf{P}) \end{split}$$

Equivalence with a Newton step.

$$\begin{split} \left[\underline{\underline{\mathbf{L}}} + \underline{\underline{\mathbf{N}}} (\underline{\dot{\mathbf{M}}}_{k}) \right] \underline{\dot{\mathbf{M}}}_{k+1} &= -\left[\underline{\mathbf{E}} + \underline{\underline{\mathbf{L}}} \, \underline{\dot{\mathbf{M}}}_{k} + \underline{\mathbf{b}} \, \Delta \mathbf{P}_{k} + \underline{\mathbf{N}} \, (\underline{\mathbf{x}}_{k}) \right] - \underline{\mathbf{b}} \, \delta (\Delta \mathbf{P}) + \underline{\underline{\mathbf{L}}} \, \underline{\dot{\mathbf{M}}}_{k} + \underline{\underline{\mathbf{N}}} (\underline{\dot{\mathbf{M}}}_{k}) \, \underline{\dot{\mathbf{M}}}_{k} \\ \left[\underline{\underline{\mathbf{L}}} + \underline{\underline{\mathbf{N}}} (\underline{\dot{\mathbf{M}}}_{k}) \right] \underline{\dot{\mathbf{M}}}_{k+1} &= -\underline{\mathbf{F}} \left(\underline{\mathbf{x}}_{k} \right) - \underline{\mathbf{b}} \, \delta (\Delta \mathbf{P}) + \left[\underline{\underline{\mathbf{L}}} + \underline{\underline{\mathbf{N}}} (\underline{\dot{\mathbf{M}}}_{k}) \right] \, \underline{\dot{\mathbf{M}}}_{k} \\ \underline{\underline{\mathbf{J}}}_{k}^{*} \, \underline{\dot{\mathbf{M}}}_{k+1} &= -\underline{\mathbf{F}} \left(\underline{\mathbf{x}}_{k} \right) - \underline{\mathbf{b}} \, \delta (\Delta \mathbf{P}) + \underline{\underline{\mathbf{J}}}_{k}^{*} \, \underline{\dot{\mathbf{M}}}_{k} \\ \underline{\underline{\mathbf{J}}}_{k}^{*} \, \left[\underline{\dot{\mathbf{M}}}_{k+1} - \underline{\dot{\mathbf{M}}}_{k} \right] &= -\underline{\mathbf{F}} \left(\underline{\mathbf{x}}_{k} \right) - \underline{\mathbf{b}} \, \delta (\Delta \mathbf{P}) \\ \underline{\underline{\mathbf{J}}}_{k}^{*} \, \delta (\underline{\dot{\mathbf{M}}}) + \underline{\mathbf{b}} \, \delta (\Delta \mathbf{P}) &= -\underline{\mathbf{F}} \left(\underline{\mathbf{x}}_{k} \right) \\ \underline{\underline{\mathbf{J}}}_{k} \, \delta \underline{\mathbf{X}} + \underline{\mathbf{b}} \, \delta (\Delta \mathbf{P}) &= -\underline{\mathbf{F}} \left(\underline{\mathbf{x}}_{k} \right) \end{split}$$

$$\begin{bmatrix} \frac{\partial \underline{\mathbf{I}}_{l}}{\partial \dot{\mathbf{M}}_{l}} & \frac{\partial \underline{\mathbf{I}}_{l}}{\partial \dot{\mathbf{M}}_{g}} & \frac{\partial \underline{\mathbf{I}}_{l}}{\partial \dot{\mathbf{M}}_{e}} & \frac{\partial \underline{\mathbf{I}}_{l}}{\partial \Delta P} \\ \frac{\partial \underline{\mathbf{I}}_{g}}{\partial \dot{\mathbf{M}}_{l}} & \frac{\partial \underline{\mathbf{I}}_{g}}{\partial \dot{\mathbf{M}}_{g}} & \frac{\partial \underline{\mathbf{I}}_{g}}{\partial \dot{\mathbf{M}}_{e}} & \frac{\partial \underline{\mathbf{I}}_{g}}{\partial \Delta P} \\ \frac{\partial \underline{\mathbf{I}}_{e}}{\partial \dot{\mathbf{M}}_{l}} & \frac{\partial \underline{\mathbf{I}}_{e}}{\partial \dot{\mathbf{M}}_{g}} & \frac{\partial \underline{\mathbf{I}}_{e}}{\partial \dot{\mathbf{M}}_{e}} & \frac{\partial \underline{\mathbf{I}}_{e}}{\partial \Delta P} \end{bmatrix}_{0} \cdot \begin{bmatrix} \Delta \dot{\mathbf{M}}_{l} \\ \Delta \dot{\mathbf{M}}_{g} \\ \Delta \dot{\mathbf{M}}_{e} \\ \Delta P \end{bmatrix} = - \begin{bmatrix} \underline{\mathbf{E}}_{l} \\ \underline{\mathbf{E}}_{g} \\ \underline{\mathbf{E}}_{e} \end{bmatrix} - \begin{bmatrix} \underline{\mathbf{I}}_{l} \\ \underline{\mathbf{I}}_{g} \\ \underline{\mathbf{I}}_{e} \end{bmatrix}_{k}$$

$$(3.24)$$

$$\begin{bmatrix} \frac{\partial \underline{\mathbf{I}}_{l}}{\partial \underline{\dot{\mathbf{M}}}_{l}} & \frac{\partial \underline{\mathbf{I}}_{l}}{\partial \underline{\dot{\mathbf{M}}}_{g}} & \frac{\partial \underline{\mathbf{I}}_{l}}{\partial \underline{\dot{\mathbf{M}}}_{e}} \\ \frac{\partial \underline{\mathbf{I}}_{g}}{\partial \underline{\dot{\mathbf{M}}}_{l}} & \frac{\partial \underline{\mathbf{I}}_{g}}{\partial \underline{\dot{\mathbf{M}}}_{g}} & \frac{\partial \underline{\mathbf{I}}_{g}}{\partial \underline{\dot{\mathbf{M}}}_{e}} \\ \frac{\partial \underline{\mathbf{I}}_{e}}{\partial \underline{\dot{\mathbf{M}}}_{l}} & \frac{\partial \underline{\mathbf{I}}_{e}}{\partial \underline{\dot{\mathbf{M}}}_{g}} & \frac{\partial \underline{\mathbf{I}}_{e}}{\partial \underline{\dot{\mathbf{M}}}_{e}} \end{bmatrix}_{0} \cdot \begin{bmatrix} \Delta \underline{\dot{\mathbf{M}}}_{l}} \\ \Delta \underline{\dot{\mathbf{M}}}_{g} \\ \Delta \underline{\dot{\mathbf{M}}}_{e} \end{bmatrix}_{k \to k+1} = -\underline{\mathbf{E}} - \underline{\mathbf{I}}_{k} - \begin{bmatrix} \frac{\partial \underline{\mathbf{I}}_{l}}{\partial \Delta P} \\ \frac{\partial \underline{\mathbf{I}}_{g}}{\partial \Delta P} \\ \frac{\partial \underline{\mathbf{I}}_{e}}{\partial \Delta P} \end{bmatrix}_{0} \Delta P_{k \to k+1}$$

$$(3.25)$$

$$\underline{\underline{\mathbf{J}}}_{0} \cdot \begin{bmatrix} \Delta \underline{\dot{\mathbf{M}}}_{l} \\ \Delta \underline{\dot{\mathbf{M}}}_{g} \\ \Delta \underline{\dot{\mathbf{M}}}_{e} \end{bmatrix}_{k \to k+1} = -\underline{\underline{\mathbf{E}}} - \underline{\underline{\mathbf{I}}}_{k} - \underline{\mathbf{p}}_{0} \Delta P_{k \to k+1} \tag{3.26}$$

$$\begin{bmatrix} \Delta \underline{\dot{\mathbf{M}}}_{l} \\ \Delta \underline{\dot{\mathbf{M}}}_{g} \\ \Delta \underline{\dot{\mathbf{M}}}_{e} \end{bmatrix}_{k \to k+1} = -\underline{\underline{\mathbf{J}}}_{0}^{-1} \left(\underline{\mathbf{E}} + \underline{\mathbf{I}}_{k} \right) - \underline{\underline{\mathbf{J}}}_{0}^{-1} \cdot \underline{\mathbf{p}}_{0} \Delta P_{k \to k+1}$$
(3.27)

$$\underline{\dot{\mathbf{M}}}_{k+1}^{n+1} - \underline{\dot{\mathbf{M}}}_{k}^{n+1} = -\underline{\mathbf{J}}_{=0}^{-1} \left(\underline{\mathbf{E}} + \underline{\mathbf{I}}_{k}\right) - \underline{\mathbf{J}}_{=0}^{-1} \cdot \underline{\mathbf{p}}_{0} \Delta P_{k \to k+1}$$

$$\underline{\dot{\mathbf{M}}}_{k+1}^{n+1} = \underline{\dot{\mathbf{M}}}_{k}^{n+1} - \underline{\mathbf{J}}_{=0}^{-1} \left(\underline{\mathbf{E}} + \underline{\mathbf{I}}_{k}\right) - \underline{\underline{\mathbf{J}}}_{0}^{-1} \cdot \underline{\mathbf{p}}_{0} \Delta P_{k \to k+1}$$

$$\underline{\dot{\mathbf{M}}}_{k}^{n+1} = \underline{\dot{\mathbf{M}}}_{k}^{n+1} - \underline{\underline{\mathbf{J}}}_{0}^{-1} \left(\underline{\mathbf{E}} + \underline{\mathbf{I}}_{k}\right) - \underline{\underline{\mathbf{J}}}_{0}^{-1} \cdot \underline{\mathbf{p}}_{0} \Delta P_{k \to k+1}$$
(3.28)

$$\underline{\dot{\mathbf{M}}}_{k+1}^{n+1} = \underbrace{-\underline{\mathbf{J}}_{0}^{-1} \cdot \underline{\mathbf{E}} + \underline{\dot{\mathbf{M}}}_{k}^{n+1} - \underline{\mathbf{J}}_{0}^{-1} \cdot \underline{\mathbf{I}}_{k}}_{\underline{\dot{\mathbf{M}}}_{*}^{n+1}} - \underbrace{\underline{\mathbf{J}}_{0}^{-1} \cdot \underline{\mathbf{P}}_{0}}_{\underline{\partial \dot{\mathbf{M}}}_{\partial \Delta P}} \Delta P_{k \to k+1}$$

$$(3.30)$$

$$\underline{\dot{\mathbf{m}}}_{k+1}^{n+1} = \underbrace{-\underline{\mathbf{J}}_{0}^{-1} \cdot \underline{\mathbf{E}} + \underline{\dot{\mathbf{m}}}_{k}^{n+1} - \underline{\mathbf{J}}_{0} \cdot \underline{\mathbf{I}}_{k}}_{\underline{\dot{\mathbf{m}}}_{*}^{n+1}} - \underbrace{\underline{\mathbf{J}}_{0}^{-1} \cdot \underline{\mathbf{p}}_{0}}_{\frac{\partial \underline{\dot{\mathbf{m}}}}{\partial \Delta P}} \Delta P_{k \to k+1}$$
(3.31)

$$\underline{\dot{\mathbf{m}}}_{k+1}^{n+1} = \underbrace{-\underline{\mathbf{J}}_{0}^{-1} \cdot \underline{\mathbf{E}} + \underline{\dot{\mathbf{m}}}_{k}^{n+1} - \underline{\mathbf{J}}_{0} \cdot \underline{\mathbf{I}}_{k}}_{\dot{\mathbf{m}}^{n+1}} - \frac{\partial \underline{\dot{\mathbf{m}}}}{\partial \Delta P} \bigg|_{0} \Delta P_{k \to k+1}$$
(3.32)

$$\underline{\dot{\mathbf{m}}}_{k+1}^{n+1} = \underbrace{-\underline{\mathbf{J}}_{0}^{-1} \cdot \underline{\mathbf{E}} + \left(\underline{\mathbf{I}} - \underline{\mathbf{J}}_{0}^{-1} \cdot \underline{\alpha}_{0}\right) \cdot \underline{\mathbf{x}}_{k}^{n+1}}_{\underline{\dot{\mathbf{m}}}_{k}^{n+1}} - \frac{\partial \underline{\dot{\mathbf{m}}}}{\partial \Delta P} \bigg|_{0} \Delta P_{k \to k+1}$$
(3.33)

$$\underline{\underline{J}}_{0} \equiv -\frac{2A_{mom}\Delta t}{\Delta z} \cdot \begin{bmatrix} K_{w,l}^{n} + \frac{K_{i,lg}^{n}}{\overline{\alpha \rho_{l}^{n}}} + \frac{1}{2} & -\frac{K_{i,lg}^{n}}{\overline{\alpha \rho_{g}^{n}}} & 0\\ -\frac{K_{w,l}^{n}}{\overline{\alpha \rho_{l}^{n}}} & K_{w,g}^{n} + \frac{K_{i,lg}^{n}}{\overline{\alpha \rho_{g}^{n}}} + \frac{K_{i,eg}^{n}}{\overline{\alpha \rho_{g}^{n}}} + \frac{1}{2} & -\frac{K_{i,eg}^{n}}{\overline{\alpha \rho_{e}^{n}}} \\ 0 & -\frac{K_{i,eg}^{n}}{\overline{\alpha \rho_{e}^{n}}} & K_{w,e}^{k} + \frac{K_{i,eg}^{n}}{\overline{\alpha \rho_{e}^{n}}} + \frac{1}{2} \end{bmatrix}$$
(3.34)

3.2.2 Linearization

The semi-implicit method, with a single Newton Step linearizes about the old time value and solves for a single delta. This has several ramifications.

3.2.2.1 Wall Drag

The beginning equation to formulate the wall drag is shown in Eqn.

$$\frac{dP}{dz}\Big|_{k}^{n+1} \equiv \left(\frac{f^{n}}{D_{h}} + \frac{K_{form}}{\Delta z}\right) \left(\frac{1}{2\rho^{n}}\right) \left(\frac{\dot{\mathbf{m}}_{k}^{n+1}}{A_{mom}}\right)^{2} \tag{3.35}$$

$$= \left[\left(\frac{f^n}{D_h} + \frac{K_{form}}{\Delta z} \right) \left(\frac{1}{2A_{mom}^2 \rho^n} \right) \right] \left[\underline{\dot{\mathbf{m}}}_{k}^{n+1} \right]^2$$
 (3.36)

$$= \left[K^n\right] \left[\underline{\dot{\mathbf{m}}}_{k}^{n+1}\right]^2 \tag{3.37}$$

$$\frac{\partial}{\partial_{\underline{\mathbf{m}}_{k}^{n+1}}} \left(\frac{dP}{dz} \Big|_{k}^{n+1} \right) = [K^{n}] 2 \left[\underline{\dot{\mathbf{m}}}_{k}^{n+1} \right]$$
(3.38)

The Momentum Equations, outlined in Section contain an implicit wall drag. This means that we need to evaluate the wall drag at the future time value. To do this in the semi-implicit

methodology requires that we linearize the future value using Newton's Method. The current implementation uses the following derivation.

Modifying this derivation to take into account the multiple Newton Steps results in the equations shown below. For brevity, the phase index, k, is dropped from this derivation. Once the linearization starts, the index, k, will refer to Newton iteration.

3.3 Structural Thermal Energy Equations

3.4 Newton's Method

COBRA currently uses a single linearized Newton step to solve the hydrodynamic equations. This method has been shown to be adequate given a small enough time step. One potential improvement that can be made to the current method is multiple Newton steps being taken with a frozen Jacobian. The Jacobian will be evaluated at the old time value and not updated during the Newton process.

3.5 Krylov Solvers

To solve a give newton iteraete, a Krylov subspace based method is used. This methodology eliminates the requirement of analytically forming the Jacobian.

Chapter 4

9:

4.1

Jacobian-Free Newton Krylov Overview

In the Jacobian-Free Newton Krylov framework, the following procedure is taken:

```
Algorithm 4.1 Transient Loop
```

```
Require: \mathbf{x}^0 and t^0
  1: Set: n = 0
 2: loop Take a Time Step
         Set: \mathbf{x}^n
 3:
         Calculate: \Delta t
 4:
         t^{n+1} := t^n + \Delta t
 5:
         Black Box: Solve for \mathbf{x}^{n+1}
 6:
 7:
         Test: CCFL

    ▷ Time-step Failure Mechanism (ccfl_fail)

         Black Box: Interfacial Area Transport Equation
 8:
```

Non-linear Function

10: **end loop** n = n + 1

Calculate: Courant Numbers

The vector function, $\underline{F}(\underline{x})$, is the nonlinear residual of the discrete version of the governing PDEs. For the physics of interest in this work, $\underline{F}(\underline{x})$ is a non-linear function. The degree of nonlinearity of $\underline{F}(\underline{x})$ depends upon the choice of numerical method used to distretize the governing PDEs. For implementational reasons, the non-linear function is broken into two parts: the explicit and the implicit portions. As shown in equation (4.1), the explicit component, \underline{E} , is independent of \underline{x} , while the implicit component, $\underline{I}(\underline{x})$, is a function of \underline{x} .

$$\underline{\mathbf{F}}(\underline{\mathbf{x}}) = \underline{\mathbf{E}} + \underline{\mathbf{I}}(\underline{\mathbf{x}}) \tag{4.1}$$

Algorithm 4.2 Modified Newton's Method - Frozen Jacobian

```
1: Define: \mathbf{x}^n
 2: Calculate: Material Properties @ \mathbf{x}^n.
 3: Calculate: Split/Merge Values @ x<sup>n</sup>.
 4: Calculate: Velocities @ x<sup>n</sup>
 5: Calculate: \underline{\mathbf{E}}_{mom}
 6: Calculate: \underline{\mathbf{E}}_{con}
 7: Set: k = 0
 8: Black Box: Predict \underline{\mathbf{x}}_k \equiv \underline{\mathbf{x}}_k^{n+1} / Apply Implicit Boundary Conditions
 9: loop Take a Newton Step
10:
            Calculate: \underline{\mathbf{I}}(\underline{\mathbf{x}}_k)_{mom}
11:
            Calculate: \underline{\mathbf{I}}(\underline{\mathbf{x}}_k)_{con}
           Black Box: Scale \underline{\mathbf{F}}(\underline{\mathbf{x}}_k) and \underline{\mathbf{J}}(\underline{\mathbf{x}}_k).
Black Box: \underline{\delta}\underline{\mathbf{x}}_k = -\mathbf{J}_0^{-1} \cdot \mathbf{F}_k
Black Box: \underline{\mathbf{x}}_{k+1}^{n+1}
12:
                                                                                                                              13:
                                                                                                        14:
           Update: Material Properties

    □ Update Variables

15:
            Test: Material Properties
16:
            Update: Junction Values
                                                                                                                          ▶ UpdateJunctions
17:
           Update: \underline{\mathbf{u}}_{k+1}^{n+1}

    ▷ CalcAxialVelocity and CalcTransVelocity

18:
           Update: \underline{\mathbf{u}}_{k+1}^*

    ▷ CalcModAxialVelocity and CalcModTransVelocity

19:
            Calculate: Convergence Norms
20:
            if Converged then
21:
                  exit loop
22:
23:
            end if
24: end loop k = k + 1
```

Solving the non-linear function depends upon finding a $\underline{\mathbf{x}}$ such that equation (4.2) is satisfied.

$$\underline{\mathbf{F}}\left(\underline{\mathbf{x}}\right) = 0\tag{4.2}$$

4.2 Newton's Method

Newton's Method for solving the nonlinear system, Equation (4.2), is an iterative process involving a multidimensional Taylor Series expansion. A first order Taylor series expansion of $\underline{\mathbf{F}}(\underline{\mathbf{x}})$ near $\underline{\mathbf{x}}_0$ is shown in equation (4.3).

$$\underline{\mathbf{F}}(\underline{\mathbf{x}}) = \underline{\mathbf{F}}(\underline{\mathbf{x}}_0 + \underline{\delta}\underline{\mathbf{x}}) = \underline{\mathbf{F}}(\underline{\mathbf{x}}_0) + \underline{\mathbf{J}}(\underline{\mathbf{x}}_0) \cdot \underline{\delta}\underline{\mathbf{x}} + \mathcal{O}(\underline{\delta}\underline{\mathbf{x}}^2)$$
(4.3)

Let $\underline{\mathbf{x}}_n$ represent a vector of known values of independent parameters, with $\underline{\mathbf{x}}_0$ being the initial conditions of the problem. Let $\underline{\delta}\underline{\mathbf{x}}_n$ be the changes in $\underline{\mathbf{x}}_n$ that will bring you from $\underline{\mathbf{x}}_n$ to $\underline{\mathbf{x}}_{n+1}$, where $\underline{\mathbf{x}}_{n+1}$ is the future time value of independent parameters.

$$\underline{\mathbf{x}}_{n+1} = \underline{\mathbf{x}}_n + \underline{\delta}\underline{\mathbf{x}}_n \tag{4.4}$$

Note that $\underline{\underline{J}}(\underline{x}_0)$ is the Jacobian of $\underline{\underline{F}}(\underline{x})$ evaluated at \underline{x}_0 . Using (4.3), equation (4.2) can be recast as a linear system where the unknown is $\underline{\delta x}$.

$$\underline{\underline{\underline{J}}}(\underline{\mathbf{x}}) \cdot \underline{\delta}\underline{\mathbf{x}} = -\underline{\underline{\mathbf{F}}}(\underline{\mathbf{x}}) \tag{4.5}$$

Solving for $\underline{\delta x}$ in (4.5) constitutes one Newton step.

4.2.1 Krylov Solver

Once (4.5) is solved for $\underline{\delta}\underline{\mathbf{x}}$, a new $\underline{\mathbf{x}}$ is obtain by equation (4.4). in order to update $\underline{\mathbf{x}}_k$ to $\underline{\mathbf{x}}_{k+1}$. To solve this linear system, a Krylov subspace method is used, in particular GMRES. We will first drop the k and k+1 subscripts because we will be using k and k+1 to denote the Krylov (inner) iteration count.

Algorithm 4.3 Newton's Method

```
1: Define: x_0
 2: Define: tolerance
 3: \gamma := 1
 4: k := 0
 5: while \gamma \leq tolerance do
                                                                                                     ▶ Test convergence of non-linear step.
            F^k := F(x^k)
                                                                                                         \triangleright Evaluate non-linear function at x^k.
            J^{k} := J(x^{k})
\delta x^{k} := J^{-k} \cdot F^{k}
                                                                                                              \triangleright Evaluate Jacobian matrix at x^k.
 7:
                                                                                \triangleright Solve for \delta x by applying the inverse of J^k to F^k.
 8:
           \begin{array}{l} \sigma x := J^{\kappa} \cdot F^{\kappa} \\ x^{k+1} := x^k + \delta x^k \\ \gamma := \min\left(\frac{\|J\delta x\|_2}{\|F\|_2}, \frac{\|\delta x\|_2}{\|x\|_2}\right) \\ k := k+1 \end{array}
                                                                                                                                          \triangleright Calculate x^{k+1}.
 9:
                                                                                                               > Calculate convergence criteria.
10:
                                                                                                                                        ▷ Increment index.
11:
12: end while
```

First, an initial guess for $\underline{\delta x}$ is chosen, $\underline{\delta x}_0$. In the literature, this initial guess is often zero for a transient simulation; the assertion is that $\underline{\delta x}$ should be small within a time step. Allowing for a nonzero initial guess, define the residual:

$$\underline{\mathbf{r}}_{0} = -\underline{\mathbf{F}}(\underline{\mathbf{x}}_{k}) - \underline{\mathbf{J}}(\underline{\mathbf{x}}_{k}) \cdot \underline{\delta}\underline{\mathbf{x}}_{0}$$

$$(4.6)$$

We now normalize the residual, $\underline{\mathbf{v}}_1 = \frac{\underline{\mathbf{r}}_0}{\|\underline{\mathbf{r}}_0\|_2}$. This vector will serve as our first basis vector (we need to start somewhere). We then enter into an iterative process starting with $\mathbf{j} = 1$. Now compute the Jacobian-vector product, $\underline{\mathbf{J}}(\underline{\mathbf{x}}_k) \cdot \underline{\mathbf{v}}_j$. We do this using a variant of Equation (4.3).

$$\underline{\mathbf{F}}(\underline{\mathbf{x}}_k + \epsilon \underline{\mathbf{y}}_j) = \underline{\mathbf{F}}(\underline{\mathbf{x}}_k + \epsilon \underline{\mathbf{J}}(\underline{\mathbf{x}}_k) \cdot \underline{\mathbf{v}}_j + \mathcal{O}((\epsilon \underline{\mathbf{v}}_j)^2)$$
(4.7)

$$\underline{\underline{\mathbf{J}}}(\underline{\mathbf{x}}_{k}) \cdot \underline{\mathbf{v}}_{j} = \frac{\underline{\mathbf{F}}(\underline{\mathbf{x}}_{k} + \epsilon \underline{\mathbf{v}}_{j}) - \underline{\mathbf{F}}(\underline{\mathbf{x}}_{k})}{\epsilon}$$
(4.8)

It is apparent that each Jacobian-vector product requires the evaluation of $\underline{F}(\underline{x})$ at a slightly perturbed value from the base state. The epsilon is a small value that is one of the tweaks that can affect convergence performance. However, traditionally this is near machine round-off.

The vector resulting from the Jacobian-Vector product, $\underline{\mathbf{w}}_j$, is then put through a Gram-Schmidt orthogonalization with all previous Krylov vectors $\underline{\mathbf{v}}_1$, $\underline{\mathbf{v}}_2$, ..., $\underline{\mathbf{v}}_{j-1}$, $\underline{\mathbf{v}}_j$. There are alternative options for this point in the algorithm (such as the Householder variation of the Arnoldi process) - these are additional options that you can change in PETSc. Part of this process (the inner-product with previous Kyrlov vectors) generates entries for the j^{th} column of a matrix, **H**. The projections of each previous Krylov vector onto $\underline{\mathbf{w}}_j$ are subtracted from $\underline{\mathbf{w}}_j$ (this is Gram-Schmidt). This new Krylov vector is determined by normalizing $\underline{\mathbf{w}}_j$, $\underline{\mathbf{v}}_{j+1} = \frac{\underline{\mathbf{w}}_j}{\|\underline{\mathbf{w}}_j\|_2}$. **Side Note:** the norm of $\underline{\mathbf{w}}_j$ is the $h_{j+1,j}$ entry in the matrix **H**.

The stopping criteria for this process is related to the norm of the latest residual, Equation (4.9), and the norm of $-\mathbf{F}(\mathbf{x}_k)$. The exact relation is determined by three tunable knobs in PETSc.

$$\|\underline{\mathbf{r}}_{j}\|_{2} = \|-\underline{\mathbf{F}} - \underline{\mathbf{J}} \cdot \underline{\delta}\underline{\mathbf{x}}_{j}\|_{2} \tag{4.9}$$

NOTE: The residual in Equation (4.9) is generated independently of constructing $\underline{\delta \mathbf{x}}_{j}$ (the final answer), which is only done at the end of the GMRES process.

After the process has stopped, a least square process is applied using $\underline{\mathbf{H}}$ to determine the coefficients for a linear combination of $\underline{\mathbf{v}}$ that will result in a $\underline{\delta}\underline{\mathbf{x}}$ that minimizes $\|-\underline{\mathbf{F}}(\underline{\mathbf{x}}_k)-\underline{\mathbf{J}}(\underline{\mathbf{x}}_k)\cdot\underline{\delta}\underline{\mathbf{x}}\|_2$. That concludes the Krlov (inner) iteration.

This $\underline{\delta \mathbf{x}}_k$ then used to computer $\underline{\mathbf{x}}_{k+1}$, which is then used in a line search (or trust region) globalization step. If good enough (PETSc options), then accept $\underline{\delta \mathbf{x}}_k$ and $\underline{\mathbf{x}}_{k+1}$ as $\underline{\delta \mathbf{x}}_n$ and $\underline{\mathbf{x}}_{n+1}$. This ends the Newton (outer) iteration.

Take next time step.

4.2.2 Globalization Strategies

4.2.2.1 Line Search

4.2.2.2 Trust Region

Appendix A: Model stuff

Test Test Test

Appendix B: Model stuff

Test Test Test

$$\begin{bmatrix} x & x & x & 0 & 0 & x - \frac{dM_g}{dP} & 0 & 0 & 0 & 0 & 0 & \frac{dM_g}{dP} \\ 0 & x & 0 & x & x & x - \frac{dM_l}{dP} & 0 & 0 & 0 & 0 & 0 & \frac{dM_g}{dP} \\ x & x & x & 0 & 0 & x - \frac{dM_g}{dP} & 0 & 0 & 0 & 0 & 0 & \frac{dM_g}{dP} + \frac{dM_g}{dP} \\ 0 & x & 0 & x & 0 & x - \frac{dM_l}{dP} - \frac{dM_e}{dP} & 0 & 0 & 0 & 0 & 0 & \frac{dM_g}{dP} + \frac{dM_g}{dP} \\ 0 & x & 0 & x & x & x - \frac{dM_e}{dP} & 0 & 0 & 0 & 0 & 0 & \frac{dM_g}{dP} + \frac{dM_g}{dP} \\ x & x & x & 0 & 0 & x - \frac{dM_l}{dP} & 0 & 0 & 0 & 0 & 0 & \frac{dM_l}{dP} \\ 0 & 0 & 0 & 0 & 0 & \frac{dM_g}{dP} & x & x & x & 0 & 0 & x - \frac{dM_g}{dP} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{dM_g}{dP} & x & x & x & 0 & 0 & x - \frac{dM_g}{dP} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{dM_g}{dP} & x & x & x & 0 & 0 & x - \frac{dM_g}{dP} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{dM_g}{dP} & x & x & x & 0 & 0 & x - \frac{dM_g}{dP} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{dM_g}{dP} & 0 & x & 0 & x & 0 & x - \frac{dM_g}{dP} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{dM_g}{dP} & 0 & x & 0 & x & 0 & x - \frac{dM_g}{dP} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{dM_g}{dP} & 0 & x & 0 & x & x & x - \frac{dM_g}{dP} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{dM_g}{dP} & 0 & x & 0 & x & x & x - \frac{dM_g}{dP} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{dM_g}{dP} & 0 & x & 0 & x & x & x - \frac{dM_g}{dP} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{dM_g}{dP} & x & x & x & 0 & 0 & x - \frac{dM_g}{dP} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{dM_g}{dP} & x & x & x & 0 & 0 & x - \frac{dM_g}{dP} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{dM_g}{dP} & x & x & x & 0 & 0 & x - \frac{dM_g}{dP} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{dM_g}{dP} & x & x & x & 0 & 0 & x - \frac{dM_g}{dP} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{dM_g}{dP} & x & x & x & 0 & 0 & x - \frac{dM_g}{dP} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{dM_g}{dP} & x & x & x & 0 & 0 & x - \frac{dM_g}{dP} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{dM_g}{dP} & x & x & x & 0 & 0 & x - \frac{dM_g}{dP} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{dM_g}{dP} & x & x & x & 0 & 0 & x - \frac{dM_g}{dP} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{dM_g}{dP} & x & x & x & 0 & 0 & x - \frac{dM_g}{dP} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{dM_g}{dP} & x & x & x & 0 & 0 & x - \frac{dM_g}{dP} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{dM_g}{dP} & x & x & x & 0 & 0 & x - \frac{dM_g}{dP} \\ 0 & 0 & 0 & 0 & 0 & 0$$

Appendix C: Model stuff

Test Test Test