Discontinuous Galerkin for Compressible and Incompressible Turbulent Flow Modelling

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Abstract

Here we describe how we can solve the Navier-Stokes, temperature and concentration equations using a shared mesh Discontinuous Galerkin (DG) method. The idea behind the approach is that it does not use indirect addressing within an element and indirect addressing only occurs between elements that are neighboring each other. In this way we obtain a method that is very fast. Here we focus on using space-time formulations with DG in space-time and adding Petrov-Galerkin stabilization terms that reduce/eliminate spurious numerical oscillations while still promoting good accuracy. This approach to reducing oscillations is mathematically rigorous and introduces non-linearity within the Petrov-Galerkin method to reduce the oscillations. The Navier Stokes and continuity equations are solved by using a pressure projection method. In addition, we attempt to remove pressure modes and ensure LBB stability by introducing similar dissipation.

Keywords: Petrov-Galerkin, oscillations, non-linearity, Navier-Stokes equations, concentration, temperature.

1. Compressible equations in conservative form

Using the conservation laws outlined above the following point-wise PDE system governing the motion of a compressible fluid is obtained

$$\frac{\partial \rho}{\partial t} + \nabla_x \cdot (\rho \mathbf{u}) = s_\rho, \tag{1}$$

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla_x \cdot (\rho \mathbf{u}\mathbf{u}) + \sigma_u \mathbf{u} = \mathbf{s}_u, \tag{2}$$

$$\frac{\partial}{\partial t}(\rho E) + \nabla_x \cdot (\rho E \mathbf{u}) = s_E, \tag{3}$$

$$\frac{\partial}{\partial t}(C) + \nabla_x \cdot (C \mathbf{u}) + \sigma_C C = s_C, \tag{4}$$

where E is the total specific energy, ρ is the density, $\mathbf{u}$ is the velocity vector, $\nabla_x = (\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z})^T$, C is a concentration field, the sources are on the r.h.s of the above equation and t is time.

2. Discretisation of momentum equations

2.1. Discretisation of inertia terms using DG

Considering a single phase the inertial terms in conservative form are:

$$\frac{\partial \hat{\rho}\mathbf{u}}{\partial t} + \nabla_x \cdot \hat{\rho}\tilde{\mathbf{u}}\mathbf{u} \tag{5}$$

and in non-conservative form:

$$\hat{\rho}\left(\frac{\partial \mathbf{u}}{\partial t} + \tilde{\mathbf{u}} \cdot \nabla_x \mathbf{u}\right) \tag{6}$$

in which $\hat{\rho} = \phi S \rho$ for porous media and $\hat{\rho} = \alpha\rho$ for inertia dominant flows. Discretising in conservative form this becomes:

$$\frac{\int_{V_e} N_i \hat{\rho}^{n+1}\mathbf{u}^{n+1} - \int_{V_e} N_i \hat{\rho}^{n}\mathbf{u}^{n}}{\Delta t} - \int_{V_e} \nabla_x N_i(\theta\hat{\rho}^{n+1}\cdot\tilde{\mathbf{u}}^{n+1}\mathbf{u}^{n+1} + (1-\theta)\hat{\rho}^{n}\cdot\tilde{\mathbf{u}}^{n}\mathbf{u}^{n})dV \tag{7}$$

$$+ \int_{\Gamma_e(\mathbf{n}\cdot\tilde{\mathbf{u}}^{n+1}<0)} N_i\theta(\hat{\rho}^{n+1}\mathbf{n}\cdot\tilde{\mathbf{u}}^{n+1}\mathbf{u}^{n+1})_{nab}d\Gamma + \int_{\Gamma_e(\mathbf{n}\cdot\tilde{\mathbf{u}}^{n}<0)} N_i(1-\theta)(\hat{\rho}^{n}\mathbf{n}\cdot\tilde{\mathbf{u}}^{n}\mathbf{u}^{n})_{nab}d\Gamma \tag{8}$$

$$+ \int_{\Gamma_e(\mathbf{n}\cdot\tilde{\mathbf{u}}^{n+1}>0)} N_i\theta\hat{\rho}^{n+1}\mathbf{n}\cdot\tilde{\mathbf{u}}^{n+1}\mathbf{u}^{n+1}d\Gamma + \int_{\Gamma_e(\mathbf{n}\cdot\tilde{\mathbf{u}}^{n}>0)} N_i(1-\theta)\hat{\rho}^{n}\mathbf{n}\cdot\tilde{\mathbf{u}}^{n}\mathbf{u}^{n}d\Gamma, \tag{9}$$

in which *nab* refers to variables associated with neighboring elements and the surface $\Gamma_e(\mathbf{n}\cdot\tilde{\mathbf{u}}^{n+1} < 0)$ is the incoming surface to element e in which $\mathbf{n}\cdot\tilde{\mathbf{u}}^{n+1} < 0$. In non-conservative form:

$$\frac{\int_{V_e} N_i \hat{\rho}^{n+\theta_\rho}\mathbf{u}^{n+1} - \int_{V_e} N_i \hat{\rho}^{n+\theta_\rho}\mathbf{u}^{n}}{\Delta t} + \int_{V_e} N_i\hat{\rho}^{n+\theta_\rho}(\theta\tilde{\mathbf{u}}^{n+1}\cdot\nabla\mathbf{u}^{n+1} + (1-\theta)\tilde{\mathbf{u}}^{n}\cdot\nabla\mathbf{u}^{n})dV \tag{10}$$

$$- \int_{\Gamma_e(\mathbf{n}\cdot\tilde{\mathbf{u}}^{n+1}<0)} N_i\theta\hat{\rho}^{n+\theta_\rho}\mathbf{n}\cdot\tilde{\mathbf{u}}^{n+1}(\mathbf{u}^{n+1} - (\mathbf{u}^{n+1})_{nab})d\Gamma \tag{11}$$

$$- \int_{\Gamma_e(\mathbf{n}\cdot\tilde{\mathbf{u}}^{n}<0)} N_i(1-\theta)\hat{\rho}^{n+\theta_\rho}\mathbf{n}\cdot\tilde{\mathbf{u}}^{n}(\mathbf{u}^{n+1} - (\mathbf{u}^{n+1})_{nab})d\Gamma. \tag{12}$$

2.2. Discretisation of momentum balance - discontinuous pressure formulation

The only difference between this formulations (as far as the momentum balance is concerned) and the continuous formulation is the treatment of pressure which is discontinuous along with saturation and density at element

boundaries. The discrete momentum balance becomes:

$$\int_{V_E} \mathbf{N}_i(\underline{\underline{\sigma}}\mathbf{u} - \nabla_x p - \mathbf{s}_u)dV + \int_{\Gamma_E} \frac{1}{2}\mathbf{N}_i\mathbf{n}(p - p_{nab})d\Gamma + \int_{\Gamma_E - \Gamma} \mathbf{N}_i\mathbf{n}(p - p_{bc})d\Gamma = 0 \tag{13}$$

and thus:

$$\mathbf{C}_{ij} = \int_{V_E} \mathbf{N}_i \nabla_x M_j dV + \int_{\Gamma_E - \Gamma} \frac{1}{2}\mathbf{N}_i\mathbf{n}M_j d\Gamma + \int_{\Gamma} \mathbf{N}_i\mathbf{n}M_j d\Gamma. \tag{14}$$

This corresponds to a central difference Discretisation for pressure on the boundaries of each finite element, that is for example:

$$\int_{V_E} \mathbf{N}_i \nabla_x p dV = -\int_{V_E} \nabla_x \mathbf{N}_i p dV + \int_{\Gamma_E} \mathbf{N}_i\mathbf{n}p_{nab}dV \tag{15}$$

$$= \int_{V_E} \mathbf{N}_i \nabla_x p dV + \frac{1}{2}\int_{\Gamma_E} \mathbf{N}_i\mathbf{n}(p - p_{nab})dV \tag{16}$$

where p_{nab} is the pressure from the neighboring element and $\mathbf{n}$ is the surface normal.

The basic momentum balance equation is obtained by using the discontinuous basis function $\mathbf{N}_i$ for velocity and M_i for pressure and in which in 3D $\mathbf{N}_i$ becomes:

$$\mathbf{N}_i = \begin{pmatrix} N_i & 0 & 0 \\ 0 & N_i & 0 \\ 0 & 0 & N_i \end{pmatrix} \tag{17}$$

The discretised force balance equation becomes:

$$\mathbf{M}_\sigma \underline{\mathbf{u}} = \mathbf{C}\underline{\mathbf{p}} + \underline{\mathbf{s}}_u. \tag{18}$$

The pressure vector is $\underline{\mathbf{p}} = (p_1\ p_2\ p_3\ ...\ p_{\mathcal{M}})^T$, the velocity vector is $\mathbf{u} = \sum_{j=1}^{\mathcal{N}} \mathbf{N}_j\mathbf{u}_j$ and $p = \sum_{j=1}^{\mathcal{M}} M_j p_j$. Also

$$\mathbf{M}_{\sigma_{ij}}^{kk} = \sum_E \int_{V_E} \mathbf{N}_i \underline{\underline{\sigma}} \mathbf{N}_j dV, \tag{19}$$

and

$$\mathbf{C}_{ij} = \sum_E \int_{V_E} \mathbf{N}_i \nabla_x M_j dV + \sum_E \int_{\Gamma_E} \frac{1}{2} \mathbf{N}_i \mathbf{n} M_j d\Gamma, \tag{20}$$

and

$$\mathbf{s}_{ui} = \sum_E \int_{V_E} \mathbf{N}_i \mathbf{s}_u dV - \sum_E \int_{\Gamma_E} \frac{1}{2} \mathbf{N}_i \mathbf{n} p_{bc} d\Gamma. \tag{21}$$

where $\mathbf{n}$ is the surface normal.

Thus, not specifying a boundary condition for pressure corresponds to a no normal flow condition which is realized through the continuity equation by weakly applying a Dirichlet no normal flow boundary condition.

3. Non-linear Petrov Galerkin methods

3.1. Compressibility

Having FEM variation of pressure allows us to simultaneously have an exact representation of the momentum balance equation as well as ensuring robustness of the the scheme e.g. positive densities from potentially complex equations of state. When using complex EoS's $\frac{\partial \tilde{\rho}_i^{n+1}}{\partial p_{\tilde{CV}_i}^{n+1}}$ is formed using a pertabation approach, that is perturbing the pressure $p_{\tilde{CV}_i}^{n+1}$ and looking how it effects the densities $\tilde{\rho}_i^{n+1}$. This avoids differentiating complex EoS's.

3.2. Pressure matrix equation

The global mass balance equation (**??**) and momentum balance equations are solved here by eliminating out velocity and solving a system of equations for pressure. The momentum balance (at time level $n+1$) and global continuity equations are:

$$\mathbf{M}_\sigma \underline{\mathbf{u}}^{n+1} = \mathbf{C} \underline{\mathbf{p}}^{n+1} + \underline{\mathbf{s}}_u^{n+1}, \tag{22}$$

$$\mathbf{M}_p \underline{\mathbf{p}}^{n+1} + \mathbf{B}^T \underline{\mathbf{u}}^{n+1} = \underline{\mathbf{s}}_p^{n+1}. \tag{23}$$

Using the discontinuous velocity within an element formulation the matrix $\mathbf{M}_\sigma$ is block diagonal and thus easily inverted - each block being local to an element. Multiplying this equation by $\mathbf{B}^T\mathbf{M}_\sigma^{-1}$ (see global continuity equation (23)) and using the global continuity equation to eliminate out $\underline{\mathbf{u}}^{n+1}$ one obtains the pressure equation:

$$(\mathbf{B}^T\mathbf{M}_\sigma^{-1}\mathbf{C} + \mathbf{M}_p)\underline{\mathbf{p}}^{n+1} = \underline{\mathbf{s}}_p^{n+1} - \mathbf{B}^T\mathbf{M}_\sigma^{-1}\underline{\mathbf{s}}_u^{n+1}. \tag{24}$$

this equation is solved for the pressure $\underline{\mathbf{p}}^{n+1}$ and then the velocity is obtained by solving equation (22).

3.3. Shock capturing

Suppose the differential equation to be solved is:

$$\mathbf{A}_{xt} \cdot \nabla_{xt}\Psi + \mathbf{H}\Psi = \mathbf{s} \tag{25}$$

in which $\mathbf{H}$ is a scattering-removal matrix operator and $\nabla_{xt} = (\frac{\partial}{\partial t}, \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z})^T$. Thus, for one dimension $\mathbf{A}_{xt} = (\mathbf{A}_t \;\; \mathbf{A}_x)^T$ and 3D $\mathbf{A}_{xt} = (\mathbf{A}_t \;\; \mathbf{A}_x \;\; \mathbf{A}_y \;\; \mathbf{A}_z)^T$ and in one dimension this equation becomes:

$$\mathbf{A}_t\frac{\partial\Psi}{\partial t} + \mathbf{A}_x\frac{\partial\Psi}{\partial x} + \mathbf{H}\Psi = \mathbf{s}. \tag{26}$$

For coupled equations the projection of $\mathbf{A}_{xt}$ onto $\nabla_{xt}\Psi$ may be written:

$$\mathbf{A}_{xt}^* = \mathbf{V}(\mathbf{A}_{xt} \cdot \nabla_{xt}\Psi)\mathbf{V}(||\nabla_{xt}\Psi||_2^2)^{-1}\nabla_{xt}\Psi. \tag{27}$$

Thus,

$$\mathbf{A}_{xt}^* \cdot \nabla_{xt}\Psi = \mathbf{A}_{xt} \cdot \nabla_{xt}\Psi \tag{28}$$

or

$$\left(\mathbf{V}(\mathbf{A}_{xt} \cdot \nabla_{xt}\Psi)\mathbf{V}(||\nabla_{xt}\Psi||_2^2)^{-1}\nabla_{xt}\Psi\right) \cdot \nabla_{xt}\Psi = \mathbf{A}_{xt} \cdot \nabla_{xt}\Psi, \tag{29}$$

in which $\mathbf{V}(\mathbf{g})$ is a diagonal matrix in which $\mathbf{V}(\mathbf{g})_{\mu\mu} = \mathbf{g}_\mu$ and the vector $||\nabla_{xt}\Psi||_2^2$ is such that the μ^{th} entry is $||\nabla_{xt}\Psi||_{2\mu}^2 = (\nabla_{xt}\Psi_\mu) \cdot (\nabla_{xt}\Psi_\mu)$. Since the matrix $\mathbf{A}_{xt}^*$ has a block diagonal structure the transport equations $\mathbf{A}_{xt}^* \cdot \nabla_{xt}\Psi + \mathbf{H}\Psi - \mathbf{s} = 0$ are a set of $\mathcal{M}$ independent scalar equations in which

the μ^{th} scalar equation is:

$$a^*_{t\,\mu}\frac{\partial \Psi_\mu}{\partial t} + a^*_{x\mu}\frac{\partial \Psi_\mu}{\partial x} + a^*_{y_\mu}\frac{\partial \Psi_\mu}{\partial y} + a^*_{z\mu}\frac{\partial \Psi_\mu}{\partial z} + \sigma_\mu \Psi_\mu = \mathbf{s}_\mu \tag{30}$$

and $a^*_{t\,\mu} = \mathbf{A}^*_{t\,\mu\mu}$, $a^*_{x\mu} = \mathbf{A}^*_{x\mu\mu}$, $a^*_{y_\mu} = \mathbf{A}^*_{y_{\mu\mu}}$, $a^*_{z\mu} = \mathbf{A}^*_{z\mu\mu}$, $\sigma_\mu = \mathbf{H}_{\mu\mu}$ and Ψ_μ is the μ^{th} scalar in the vector Ψ. In equation (109) it is assumed that $\mathbf{H}$ is a diagonal. If it is not then the system of equations can be easily manipulated so as to diagonalise $\mathbf{H}$, see equations (45), (46), (47), (48). Since the equations have been uncoupled then the scalar equation methods described in the previous section can now be applied. This is effectively done below.

The Petrov-Galerkin's modified form of the differential equation is:

$$(\mathbf{I} - (\nabla_{xt} \cdot \mathbf{A}^*_{xt})^T \mathbf{P}^*_{xt})(\mathbf{A}_{xt} \cdot \nabla_{xt}\Psi + \mathbf{H}\Psi - \mathbf{s}) = \mathbf{0}, \tag{31}$$

or equvilently from equation (28) :

$$(\mathbf{I} - (\nabla_{xt} \cdot \mathbf{A}^*_{xt})^T \mathbf{P}^*_{xt})(\mathbf{A}^*_{xt} \cdot \nabla_{xt}\Psi + \mathbf{H}\Psi - \mathbf{s}) = \mathbf{0}. \tag{32}$$

Testing equation (32) with a diagonal matrix of space-time basis function $\mathbf{N}_{xti}$ (this has the basis function N_{xti} along its main diagonal), integrating over a single element V_E and applying integration by parts results in:

$$\int_{V_E} \mathbf{N}_{xti}\mathbf{r}dV_{xt} - \int_{\Gamma_E} \mathbf{N}_{xti}(\mathbf{n}_{xt} \cdot \mathbf{A}_{xt})^-(\Psi - \Psi_{bc})d\Gamma_{xt} \tag{33}$$

$$+ \int_{V_E} ((\nabla_{xt}\mathbf{N}_{xti}) \cdot \mathbf{A}^*_{xt})^T \mathbf{P}^*_{xt}\mathbf{r}dV_{xt} + \int_{\Gamma_E} \mathbf{N}_{xti}\mathbf{n}_{xt} \cdot \mathbf{A}^*_{xt}\mathbf{P}^*_{xt}\mathbf{r}d\Gamma_{xt} = \mathbf{0}, \tag{34}$$

with a finite element expansion $\Psi = \sum_{j=1}^{\mathcal{N}} \mathbf{N}_{xtj}\mathbf{\Psi}_j$ (where $\mathbf{\Psi}_j$ is the order $\mathcal{M}$ vector of unknowns at node j) and $\mathbf{r} = \mathbf{A}_{xt} \cdot \nabla_{xt}\Psi + \mathbf{H}\Psi - \mathbf{s}$. Using the eigen-decomposition $\mathbf{n}_{xt} \cdot \mathbf{A}_{xt} = \mathbf{L}_{xt}\mathbf{\Lambda}_{xt}\mathbf{R}_{xt}$ then $(\mathbf{n}_{xt} \cdot \mathbf{A}_{xt})^- = \mathbf{L}_{xt}\mathbf{\Lambda}^-_{xt}\mathbf{R}_{xt}$ with $\mathbf{\Lambda}^-_{xtkk} = \min\{0, \mathbf{\Lambda}_{xtkk}\}$. This eigen decomposition enables the boundary condition to be applied to incoming information only. We apply a zero boundary condition for the residual $\mathbf{r} = \mathbf{0}$ which results in:

$$\int_{V_E} \mathbf{N}_{xti}\mathbf{r}dV_{xt} - \int_{\Gamma_E} \mathbf{N}_{xti}(\mathbf{n}_{xt}\cdot\mathbf{A}_{xt})^{-}(\Psi-\Psi_{bc})d\Gamma_{xt} \tag{35}$$

$$+\int_{V_E}((\nabla_{xt}\mathbf{N}_{xti})\cdot\mathbf{A}^*_{xt})^T\mathbf{P}^*_{xt}\mathbf{r}dV_{xt} = \mathbf{0}. \tag{36}$$

$\mathbf{P}^*_{xt}$ is a function of $\mathbf{A}^*_{xt}$ and the size and shape of the elements, for example:

$$\mathbf{P}^*_{xt} = \frac{1}{4}(|\mathbf{A}^*_{xt}\cdot\nabla_{xt}\mathbf{N}_{xti}|)^{-1}, \tag{37}$$

or using the 2 matrix norm and the space-time Jacobian matrix $\mathbf{J}_{xt}$:

$$\mathbf{P}^*_{xt} = \frac{1}{4}(||\mathbf{J}^{-1}_{xt}\mathbf{A}^*_{xt}||_2)^{-1}. \tag{38}$$

Since the matrices $\mathbf{A}^*_t$, $\mathbf{A}^*_x$, $\mathbf{A}^*_y$, $\mathbf{A}^*_z$ that go to make up

$$\mathbf{A}^*_{xt} = (\mathbf{A}^{*T}_t, \mathbf{A}^{*T}_x, \mathbf{A}^{*T}_y, \mathbf{A}^{*T}_z)^T \tag{39}$$

are diagonal the matrix $\mathbf{P}^*_{xt}$ is also diagonal. In the traditional Petrov Galerkin method $\mathbf{A}^*_{xt} = \mathbf{A}_{xt}$ in the above and $\mathbf{P}_{xt}$ replaces $\mathbf{P}^*_{xt}$. The finite element space-time Jacobian matrix for 3D time dependent problems is:

$$\mathbf{J}_{xt} = \begin{pmatrix} \mathbf{I}\frac{\partial t}{\partial t'} & \mathbf{I}\frac{\partial x}{\partial t'} & \mathbf{I}\frac{\partial y}{\partial t'} & \mathbf{I}\frac{\partial z}{\partial t'} \\ \mathbf{I}\frac{\partial t}{\partial x'} & \mathbf{I}\frac{\partial x}{\partial x'} & \mathbf{I}\frac{\partial y}{\partial x'} & \mathbf{I}\frac{\partial z}{\partial x'} \\ \mathbf{I}\frac{\partial t}{\partial y'} & \mathbf{I}\frac{\partial x}{\partial y'} & \mathbf{I}\frac{\partial y}{\partial y'} & \mathbf{I}\frac{\partial z}{\partial y'} \\ \mathbf{I}\frac{\partial t}{\partial z'} & \mathbf{I}\frac{\partial x}{\partial z'} & \mathbf{I}\frac{\partial y}{\partial z'} & \mathbf{I}\frac{\partial z}{\partial z'} \end{pmatrix}, \tag{40}$$

where the variables with $'$ are the local variables and where $\mathbf{I}$ is the $\mathcal{M}\times\mathcal{M}$ identity matrix in which $\mathcal{M}$ is the number solution variables at each DG node. For uniform space-time resolution with a time step size of Δt and an element size of Δx (in the x-direction), Δy (in the y-direction), Δz (in the z-direction), then:

$$\mathbf{J}_{xt} = \begin{pmatrix} \mathbf{I}\frac{1}{2}\Delta t & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{I}\frac{1}{2}\Delta x & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{I}\frac{1}{2}\Delta y & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{I}\frac{1}{2}\Delta z \end{pmatrix}. \tag{41}$$

In a similar way to the scalar equation, the value of $\mathbf{P}^*_{xt}$ can be adjusted to ensure that the resulting value of $\mathbf{P}^*_{xt}$ is not so large that there is more transport backwards than forwards in the resulting discrete system of equations by:

$$\mathbf{P}^*_{xt} = \min\{(\mathbf{H}^* + \mathbf{E})^{-1}, \frac{1}{4}(||\mathbf{J}^{-1}_{xt}\mathbf{A}^*_{xt}||_2)^{-1}\}. \tag{42}$$

in which the diagonal entries of the matrix $\mathbf{H}^*$ could for example be:

$$\mathbf{H}^* = (\mathbf{H}^T\mathbf{H})^{\frac{1}{2}} \tag{43}$$

and $\mathbf{E}$ contains small positive numbers to avoid dividing by zero or near zero when one or more of the diagonals of $\mathbf{H}^*$ is zero or very small e.g. 1×10^{-10}. A simpler approach is to use a diagonal matrix $\mathbf{H}^*$ and define it with:

$$\mathbf{H}^*\Psi = \mathbf{H}\Psi \tag{44}$$

and

$$\mathbf{H}^* = \frac{\mathbf{H}\Psi}{\Psi}. \tag{45}$$

If $\mathbf{H}^*$ has positive diagonal elements then there is a net absorption of the field associated with that diagonal else there is a net positive source and thus either:

$$\mathbf{H}^* = \left|\frac{\mathbf{H}\Psi}{\Psi}\right|, \tag{46}$$

or

$$\mathbf{H}^* = \max\left\{\frac{\mathbf{H}\Psi}{\Psi}, \mathbf{0}\right\}. \tag{47}$$

The latter is less invasive and thus preferred. This approach may also be used with a source term $\mathbf{s}$ using:

$$\mathbf{H}^* = \max\left\{\frac{\mathbf{H}\Psi - \mathbf{s}}{\Psi}, \mathbf{0}\right\}. \tag{48}$$

In the above we can work with the stabilization in diffusion form with:

$$\int_{V_E} \mathbf{N}_{xti}\mathbf{r}dV_{xt} - \int_{\Gamma_E} \mathbf{N}_{xti}(\mathbf{n}_{xt}\cdot\mathbf{A}_{xt})^{-}(\Psi-\Psi_{bc})d\Gamma_{xt} \tag{49}$$

$$+\int_{V_E} (\nabla_{xt}\mathbf{N}_{xti})^T\mathbf{K}_{2h}\nabla_{xt}\Psi dV_{xt} = \mathbf{0}, \tag{50}$$

in which the $\mathcal{M}\times\mathcal{M}$ diagonal matrix containing the diffusion coefficients is:

$$\mathbf{K}_{2h} = \mathbf{A}_{xt}^{*T}\mathbf{P}_{xt}^{*}\mathbf{A}_{xt}^{*}, \tag{51}$$

or simplifying this equation:

$$\mathbf{K}_{2h} = \mathbf{V}(\mathbf{A}_{xt}\cdot\nabla_{xt}\Psi)\mathbf{P}_{xt}^{*}\mathbf{V}(||\nabla_{xt}\Psi||_2^2)^{-1}\mathbf{V}(\mathbf{A}_{xt}\cdot\nabla_{xt}\Psi). \tag{52}$$

The resulting diagonal matrix $\mathbf{K}_{2h}$ is positive semi-definite. Alternatively one can work with the residual only, by replacing $\mathbf{A}_{xt}\cdot\nabla_{xt}\Psi$ with the residual $\mathbf{r}$, which results in:

$$\mathbf{K}_{2h} = \mathbf{V}(\mathbf{r})^T\mathbf{P}_{xt}^{*}\mathbf{V}(||\nabla_{xt}\Psi||_2^2)^{-1}\mathbf{V}(\mathbf{r}) \tag{53}$$

which is always positive because $\mathbf{P}_{xt}^{*}$ is positive semi-definite (as well as diagonal) and in which $\mathbf{V}(\mathbf{r})$ is the diagonal matrix containing the residual of the governing equations on its diagonal. Equation (117) for the diffusivity can be derived by re-defining $\mathbf{A}_{xt}^{*}$ in equation (106) to:

$$\mathbf{A}_{xt}^{*} = \mathbf{V}(\mathbf{r})\mathbf{V}(||\nabla_{xt}\Psi||_2^2)^{-1}\nabla_{xt}\Psi. \tag{54}$$

3.3.1. Simplified coupled equations and θ-time stepping

Assuming time is discretised using the two level θ-method:

$$\mathbf{r} = \mathbf{A}_t\frac{\Psi^{n+1}-\Psi^n}{\Delta t} + \mathbf{A}\cdot\nabla\Psi^{n+\theta} + \mathbf{H}\Psi^{n+\theta} - \mathbf{s}^{n+\theta}, \tag{55}$$

with $\mathbf{A} = (\mathbf{A}_x \;\; \mathbf{A}_y \;\; \mathbf{A}_z)^T$ and $\Psi^{n+\theta} = \Theta\Psi^{n+1} + (\mathbf{I}-\Theta)\Psi^n$ in which Θ is a diagonal matrix containing the time stepping parameters and also defining

$$\nabla_{xt}\Psi = \left(\frac{\Psi^{n+1}-\Psi^n}{\Delta t},\; (\nabla\Psi^{n+\theta})^T\right)^T. \tag{56}$$

Using this definition (equation (56)) enables the application of the mechanics of space-time discretisation, developed here, for example:

$$\mathbf{A}^*_{xt} = (\mathbf{A}^{*T}_t,\ \mathbf{A}^{*T})^T = \mathbf{V}(\mathbf{A}_{xt} \cdot \nabla_{xt}\Psi)\mathbf{V}(||\nabla_{xt}\Psi||^2_2)^{-1}\nabla_{xt}\Psi. \tag{57}$$

By applying diffusion only in Cartesian space the stabilized discrete equations in diffusion form can be written:

$$\int_{V_E} \mathbf{N}_i \mathbf{r} dV - \int_{\Gamma_E} \mathbf{N}_i (\mathbf{n} \cdot \mathbf{A})^- (\Psi^{n+\theta} - \Psi^{n+\theta}_{bc}) d\Gamma + \int_{V_E} (\nabla \mathbf{N}_i)^T \mathbf{K} \nabla \Psi^{n+1} dV = \mathbf{0}. \tag{58}$$

3.3.2. Time Discretisation

A new time discretisation method is developed here. When high order discretisation in time is sought then the method is based on Crank-Nicholson or higher order time stepping. The Crank-Nicholson method was chosen, because it has the simplicity of a two level time stepping method, is unconditionally stable and second order accurate. Moreover, the use of time steps of the order of the grid Courant number and above can result in numerical oscillations and unphysical solutions. Thus, a parameter θ is introduced, in which $\theta = 0$ corresponds to the forward Euler time stepping method, $\theta = \frac{1}{2}$ corresponds to the Crank-Nicholson time stepping method and $\theta = 1$ backward-Euler. Then the time stepping takes the form the temperature advection-diffusion equation:

$$\int N_i \left(\frac{T^{n+1}_i - T^n_i}{\Delta t} - s \right) dV =$$

$$\int \nabla N_i \cdot \left(\theta(\mathbf{a}^{n+1}\widetilde{T}^{n+1} + k^{n+1}\nabla\widetilde{T}^{n+1}) + (1-\theta)(\mathbf{a}^n\widetilde{T}^n + k^n\nabla\widetilde{T}^n) \right) dV +$$

$$\int_{\Gamma_E} N_i \left[\theta \left(\mathbf{a}^{n+1} \cdot \mathbf{n}\widetilde{T}^{n+1} + \mathbf{n} \cdot k^{n+1}\nabla\widetilde{T}^{n+1} \right) + (1-\theta) \left(\mathbf{a}^n \cdot \mathbf{n}\widetilde{T}^n + \mathbf{n} \cdot k^n\nabla\widetilde{T}^n \right) \right] d\Gamma \tag{59}$$

or simplifying using the flux

$$\mathbf{h}^n = \mathbf{a}\widetilde{T}^n + k^n\nabla\widetilde{T}^n \tag{60}$$

to obtain:

$$\int N_i \left(\frac{T_i^{n+1} - T_i^n}{\Delta t} - s \right) dV =$$
$$\int \nabla N_i \cdot \left(\theta \mathbf{h}^{n+1} + (1-\theta)\mathbf{h}^n \right) dV +$$
$$\int_{\Gamma_E} N_i \mathbf{n} \cdot \left(\theta \mathbf{h}^{n+1} + (1-\theta)\,\mathbf{h}^n \right) d\Gamma \tag{61}$$

in which ∇N_i is very much analogous to the normal to the element $\mathbf{n}$. For each time step a value of θ is calculated at each element face based on the satisfaction of a TVD criteria. In 1-D, assuming the simplest element type with constant basis functions N_i across an element ($i = E$) and assuming the flux limiting values of the flux at the $i - \frac{1}{2}$ and $i + \frac{1}{2}$ boundaries are $h^n_{i-\frac{1}{2}}$ and $h^n_{i+\frac{1}{2}}$ at time level n, the time discretization becomes:

$$\Delta x_i \left(\frac{T_i^{n+1} - T_i^n}{\Delta t} \right) = \theta^{n+\frac{1}{2}}_{i-\frac{1}{2}} h^{n+1}_{i-\frac{1}{2}} + (1-\theta^{n+\frac{1}{2}}_{i-\frac{1}{2}}) h^n_{i-\frac{1}{2}} - \theta^{n+\frac{1}{2}}_{i+\frac{1}{2}} h^{n+1}_{i+\frac{1}{2}} - (1-\theta^{n+\frac{1}{2}}_{i+\frac{1}{2}}) h^n_{i+\frac{1}{2}} \tag{62}$$

with

$$h^n_{i-\frac{1}{2}} = a^n_{i-\frac{1}{2}} T^n_{i-\frac{1}{2}} + k^n_{i-\frac{1}{2}} \frac{\partial T^n}{\partial x} \Big|_{i-\frac{1}{2}}$$

Δx_i is the width of the E^{th} element and $\theta^{n+\frac{1}{2}}_{i+\frac{1}{2}}$ is the value of θ associated with face $i + \frac{1}{2}$ and the time step from time level n to $n+1$. The representation of $k^n_{i-\frac{1}{2}} \frac{\partial T^n}{\partial x}|_{i-\frac{1}{2}}$ is considered in a following section.

Re-arranging Eqn. (62):

$$\left(\Delta x_i - \Delta t \frac{\left[-\widehat{\theta}^{n+\frac{1}{2}}_{i-\frac{1}{2}} (-h^{n+1}_{i-\frac{1}{2}} + h^n_{i-\frac{1}{2}}) + \widehat{\theta}^{n+\frac{1}{2}}_{i+\frac{1}{2}} (-h^{n+1}_{i+\frac{1}{2}} + h^n_{i+\frac{1}{2}}) \right]}{T_i^{n+1} - T_i^n} \right) \left(\frac{T_i^{n+1} - T_i^n}{\Delta t} \right) =$$
$$h^{n+1}_{i-\frac{1}{2}} - h^{n+1}_{i+\frac{1}{2}}$$

with

$$\widehat{\theta}^{n+\frac{1}{2}}_{i-\frac{1}{2}} = 1 - \theta^{n+\frac{1}{2}}_{i-\frac{1}{2}}.$$

Now since backward Euler time stepping is TVD in the same way that first

order upwind scheme is spatially, a positive definite mass matrix is a sufficient condition for the backward Euler scheme above to be TVD (see **?**). Thus, the diagonal mass matrix (the term in brackets) must be non-negative, after re-arranging this requirement becomes

$$\frac{\Delta t}{\Delta x_i \left(T_i^{n+1} - T_i^n\right)} \left[\widehat{\theta}_{i-\frac{1}{2}}^{n+\frac{1}{2}} \left(h_{i-\frac{1}{2}}^n - h_{i-\frac{1}{2}}^{n+1}\right) - \hat{\theta}_{i+\frac{1}{2}}^{n+\frac{1}{2}} \left(h_{i+\frac{1}{2}}^n - h_{i+\frac{1}{2}}^{n+1}\right)\right] \leq 1$$

and thus

$$\left(\widehat{\theta}_{i-\frac{1}{2}}^{n+\frac{1}{2}} p_{i-\frac{1}{2}}^{n+\frac{1}{2}} - \widehat{\theta}_{i+\frac{1}{2}}^{n+\frac{1}{2}} q_{i+\frac{1}{2}}^{n+\frac{1}{2}}\right) \leq 1$$

with

$$p_{i-\frac{1}{2}}^{n+\frac{1}{2}} = \left(\frac{h_{i-\frac{1}{2}}^n - h_{i-\frac{1}{2}}^{n+1}}{T_i^{n+1} - T_i^n}\right) \frac{\Delta t}{\Delta x_i} \quad \text{and} \quad q_{i+\frac{1}{2}}^{n+\frac{1}{2}} = \left(\frac{h_{i+\frac{1}{2}}^n - h_{i+\frac{1}{2}}^{n+1}}{T_i^{n+1} - T_i^n}\right) \frac{\Delta t}{\Delta x_i}$$

which is satisfied if

$$-\widehat{\theta}_{i-\frac{1}{2}}^{n+\frac{1}{2}} p_{i-\frac{1}{2}}^{n+\frac{1}{2}} \leq \frac{1}{2} \quad \text{and} \quad -\widehat{\theta}_{i-\frac{1}{2}}^{n+\frac{1}{2}} q_{i-\frac{1}{2}}^{n+\frac{1}{2}} \geq \frac{1}{2} \tag{63}$$

Thus, to make the value of $\theta_{i-\frac{1}{2}}^{n+\frac{1}{2}} = 1 - \widehat{\theta}_{i-\frac{1}{2}}^{n+\frac{1}{2}}$ as close to θ_{aim} as possible we choose

$$\theta_{i-\frac{1}{2}}^{n+\frac{1}{2}} = \max\left\{\theta_{aim}, 1 - \beta \min\left\{\left|\frac{1}{p_{i-\frac{1}{2}}^{n+\frac{1}{2}}}\right|, \left|\frac{1}{q_{i-\frac{1}{2}}^{n+\frac{1}{2}}}\right|\right\}\right\}$$

with $\beta = \frac{1}{2}$ and $\theta_{aim} = \frac{1}{2}$ is the base scheme and is the high order accurate Crank Nicholson scheme and $\theta_{aim} = 0$ if it is forward Euler time stepping which is favored when interface capturing.

3.3.3. Multi-dimensional temporal limiting between elements

The high resolution θ method can be extended to multi-dimensions by replacing $h_{i-\frac{1}{2}}^n$ with the integral of $\tilde{h}_f^n$ over face f and Δx_i replaced by the volume L_i (contribution from diagonal mass matrix) of the i^{th} node. Using similar arguments to the 1-D case the following expression for $\theta_f^{n+\frac{1}{2}}$ of face f

is obtained:

$$\theta_f^{n+\frac{1}{2}} = \max\left\{\theta_{aim}, 1-\beta\min\left\{\left|\frac{1}{p_f^{n+\frac{1}{2}}}\right|, \left|\frac{1}{q_f^{n+\frac{1}{2}}}\right|\right\}\right\} \tag{64}$$

with

$$p_f^{n+\frac{1}{2}} = \frac{g_f^{n+\frac{1}{2}}\Delta t}{(T_c^{n+1}-T_c^n)L_c} \quad \text{and} \quad q_f^{n+\frac{1}{2}} = \frac{g_f^{n+\frac{1}{2}}\Delta t}{(T_d^{n+1}-T_d^n)L_d} \tag{65}$$

and

$$g_f^{n+\frac{1}{2}} = (\tilde{h}_f^n - \tilde{h}_f^{n+1}). \tag{66}$$

Elements c and d in these equations refer to the two elements that are adjacent to face f. Extensions of this method to differential equations with time-dependent terms like $\frac{\partial \rho T}{\partial t}$ are realized by replacing, in Eqn. (65), T_j^n and T_j^{n+1} by $T_j^n\rho_j^n$ and $T_j^{n+1}\rho_j^{n+1}$ respectively for $j=c$ and $j=d$. In addition, this expression (66) is also used for high order elements but it this case the lengths L_c and L_d are evaluated normal to the element face and are the resolution length scale normal to the face e.g. found from the gradients of the shape functions normal to the face. Also for calculating θ, within an element, the approach in the section below is followed. It may also be generalized to include the jump conditions.

3.3.4. Automatic spatially variable θ choice within an element or at the differential equation level

In transient modelling there will be conflicting demands on θ from accuracy ($\theta = \frac{1}{2}$ for second order accuracy) to robustness and use of large time steps ($\theta = 1$). Thus there is a need to autmoaticaly choose θ and allow it to vary spatially.

Here we use a simple method based on the observation that as long as a discretised transport equation can be written in the form:

$$M_{tran}\frac{\underline{T}^{n+1}-\underline{T}^n}{\Delta t} + A_{tran}\underline{T}^{n+1} = 0 \tag{67}$$

using θ time stepping and a modified positive definite mass matrix M_{mod} then the time stepping method will be Total Variation Diminishing (TVD)

in time and the transport discretised equation with θ differencing is:

$$M_{mod}\frac{\underline{T}^{n+1}-\underline{T}^{n}}{\Delta t}+A_{tran}\underline{T}^{n+1}=0. \tag{68}$$

This may be the discrete equations within an element for example or across all elements. Now to map this system to nodal solution variables one simply:

$$\frac{\underline{T}^{n+1}-\underline{T}^{n}}{\Delta t}+M_{mod}^{-1}A_{tran}\underline{T}^{n+1}=0, \tag{69}$$

or

$$\frac{\underline{T}^{n+1}-\underline{T}^{n}}{\Delta t}+\underline{S}^{n+1}=0. \tag{70}$$

This may provide the nodal variables and the approach below can be applied to determine θ by using the expansions $T^n=\sum_j N_j T_j^n$ and $S^n=\sum_j N_j S_j^n$. This approach can also be used to form the jump conditions at element boundaries but at the interface this approach will result in two values of θ so one simply uses the value of θ closest to 1.

To simplify the analysis and ensure that this condition is satisfied the same condition can be applied to the equation point wise (at every quadrature point in practice) as long as the equation does not contain spatial derivatives - the case for the free surface. The point-wise enforcement may result in a conservative value of θ. That is:

$$(1+f)\frac{T^{n+1}-T^{n}}{\Delta t}+S^{n+1}=0 \tag{71}$$

for positive $(1+f)$ and source term at time level n of S^n. As in all of this document the value of θ is assumed to be that between time levels n and $n+1$ and thus may have a superscript of $n+\frac{1}{2}$ which is implied in this work but omitted for simplicity. Comparing with θ discretisation of the r.h.s. variable S:

$$\frac{T^{n+1}-T^{n}}{\Delta t}+\theta S^{n+1}+(1-\theta)S^{n}=0 \tag{72}$$

it is seen that

$$f=(1-\theta)\frac{\Delta t(-S^{n+1}+S^{n})}{(T^{n+1}-T^{n})}=(1-\theta)q^{n+\frac{1}{2}} \tag{73}$$

which defines the variable

$$q^{n+\frac{1}{2}} = \frac{\Delta t(-S^{n+1} + S^n)}{(T^{n+1} - T^n)}, \tag{74}$$

and thus the condition $1 + f \geq 0$ becomes a condition on θ:

$$-(1-\theta)q^{n+\frac{1}{2}} \leq 1. \tag{75}$$

To ensure θ is as close to $\frac{1}{2}$ (for accuracy) while still satisfying condition (75) point wise:

$$\theta = 1 - \frac{1}{\max\{2, -q^{n+\frac{1}{2}}\}}. \tag{76}$$

From this equation and the definition of $q^{n+\frac{1}{2}}$ it is easy to see that θ will be close or equal to $\frac{1}{2}$ if either Δt is small or $(-S^{n+1} + S^n)$ is small relative to $(T^{n+1} - T^n)$. It also needs to be applied as part of an iterative procedure within a time step, for example starting with $\theta = 1$ on the first iteration or with a guess of $q^{n+\frac{1}{2}}$.

3.3.5. Extension of θ-method to three or more time levels

The θ-method is easily extended to a general three level (or more) time stepping method:

$$\frac{\hat{a}T^{n+1} + \hat{b}T^n + \hat{c}T^{n-1}}{\Delta t} + \hat{d}S^{n+1} + \hat{e}S^n + \hat{f}S^{n-1} = 0, \tag{77}$$

for coefficients $\hat{a}$, $\hat{b}$, $\hat{c}$, $\hat{d}$, $\hat{e}$, $\hat{f}$ which define the time stepping scheme. Rearranging equation (72) and comparing with this equation (77) for θ one obtains:

$$1 - \theta = \frac{(\hat{a}-1)\tilde{T}^{n+1} + (\hat{b}+1)T^n + \hat{c}T^{n-1}}{\Delta t(-\tilde{S}^{n+1} + S^n)} + \frac{(\hat{d}-1)\tilde{S}^{n+1} + \hat{e}S^n + \hat{f}S^{n-1}}{-\tilde{S}^{n+1} + S^n} \tag{78}$$

where $\tilde{T}^{n+1}$, $\tilde{S}^{n+1}$ is used in the future variables as these are not known but need to be approximated by for example iterating on the above scheme. The TVD criteria in time is met by adjusting this value of θ (minimally in some

sense) so that (75) holds. For example, if (75) does not hold then set

$$\theta = 1 - \frac{1}{\max\{1, -q^{n+\frac{1}{2}}\}}. \tag{79}$$

For stability it may be benefitical to limit the value of $\theta \in [0, 1]$.

3.3.6. Navier Stokes equations

The momentum balance equations plus continuity can be define with

$$A_t = \begin{pmatrix} \rho & 0 & 0 & 0 \\ 0 & \rho & 0 & 0 \\ 0 & 0 & \rho & 0 \\ 0 & 0 & 0 & \frac{\partial \rho}{\partial p} \end{pmatrix}, \tag{80}$$

$$A_x = \begin{pmatrix} \rho u & 0 & 0 & 1 \\ 0 & \rho u & 0 & 0 \\ 0 & 0 & \rho u & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \tag{81}$$

$$A_y = \begin{pmatrix} \rho v & 0 & 0 & 1 \\ 0 & \rho v & 0 & 0 \\ 0 & 0 & \rho v & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \tag{82}$$

$$A_z = \begin{pmatrix} \rho w & 0 & 0 & 1 \\ 0 & \rho w & 0 & 0 \\ 0 & 0 & \rho w & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \tag{83}$$

in which the solution vector is $\Psi = (u \;\; v \;\; w \;\; p)^T$.

The above matrices are used with the above theory which results in a diffusion matrix for each each variable. However, we set the diffusion for pressure to zero so as not to compromise conservation of mass and other advected variables. Even when we solve the governing equations in conservative form we form the above matrices in order to from the resulting diffusion.

3.3.7. Concentration or Energy Equations

The concentration equation for one component C ignoring the coupling of the components as far as the dissipation is concerned is:

$$A_t = \rho, \tag{84}$$

$$A_x = \rho u, \tag{85}$$

$$A_y = \rho v, \tag{86}$$

$$A_z = \rho w, \tag{87}$$

in which the solution vector is $\Psi = C$.

4. Petrov-Galerkin - fourth order dissipation

High order dissipation may be preferential especially if one is using high order elements - quadratic or above. The idea is that this type of dissipation is more scale selective than lower order dissipation. That is it does something similar to diffusion for short wave length oscillations but does not influence much long wavelengths.

For coupled equations the projection of $\mathbf{A}_{xt}$ onto

$$\nabla^2_{xt}\Psi = \frac{\partial^2\Psi}{\partial t^2} + \frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} + \frac{\partial^2\Psi}{\partial z^2} \tag{88}$$

may be written:

$$\mathbf{B}^*_{xt} = \mathbf{V}(\mathbf{A}_{xt}\cdot\nabla_{xt}\Psi)\mathbf{V}(||\nabla^2_{xt}\Psi||^2_2)^{-1}\mathbf{V}(\nabla^2_{xt}\Psi). \tag{89}$$

Thus,

$$\mathbf{B}^*_{xt}\nabla^2_{xt}\Psi = \mathbf{A}_{xt}\cdot\nabla_{xt}\Psi \tag{90}$$

or

$$\left(\mathbf{V}(\mathbf{A}_{xt}\cdot\nabla_{xt}\Psi)\mathbf{V}(||\nabla^2_{xt}\Psi||^2_2)^{-1}\mathbf{V}(\nabla^2_{xt}\Psi)\right)\nabla^2_{xt}\Psi=\mathbf{A}_{xt}\cdot\nabla_{xt}\Psi. \tag{91}$$

in which $\mathbf{V}(\mathbf{g})$ is a diagonal matrix in which $\mathbf{V}(\mathbf{g})_{\mu\mu}=\mathbf{g}_\mu$ and the vector $\nabla^2_{xt}\Psi$ is such that the μ^{th} entry is $(\nabla^2_{xt}\Psi)_\mu=\nabla^2_{xt}\Psi_\mu$. Since the matrix $\mathbf{B}^*_{xt}$ has a diagonal structure the transport equations $\mathbf{B}^*_{xt}\nabla^2_{xt}\Psi+\mathbf{H}\Psi-\mathbf{s}=0$ are a set of $\mathcal{M}$ independent scalar equations in which the μ^{th} scalar equation is:

$$b^*_{xt\mu}\left(\frac{\partial^2\Psi_\mu}{\partial t^2}+\frac{\partial^2\Psi_\mu}{\partial x^2}+\frac{\partial^2\Psi_\mu}{\partial y^2}+\frac{\partial^2\Psi_\mu}{\partial z^2}\right)+\sigma_\mu\Psi_\mu=\mathbf{s}_\mu \tag{92}$$

and $b^*_{xt\mu}=\mathbf{B}^*_{xt\mu\mu}$, $\sigma_\mu=\mathbf{H}_{\mu\mu}$ and Ψ_μ is the μ^{th} scalar in the vector Ψ. In equation (109) it is assumed that $\mathbf{H}$ is a diagonal. If it is not then the system of equations can be easily manipulated so as to diagonalise $\mathbf{H}$, see equations (45), (46), (47), (48). Since the equations have been uncoupled then the scalar equation methods described in the previous section can now be applied. This is effectively done below.

The Hyper-Petrov-Galerkin's modified form of the differential equation is:

$$(\mathbf{I}+\nabla^2_{xt}\mathbf{B}^*_{xt}\mathbf{P}^*_{xt})(\mathbf{A}_{xt}\cdot\nabla_{xt}\Psi+\mathbf{H}\Psi-\mathbf{s})=\mathbf{0}, \tag{93}$$

or equivalently from equation (90):

$$(\mathbf{I}+\nabla^2_{xt}\mathbf{B}^*_{xt}\mathbf{P}^*_{xt})(\mathbf{B}^*_{xt}\nabla^2_{xt}\Psi+\mathbf{H}\Psi-\mathbf{s})=\mathbf{0}. \tag{94}$$

Testing equation (93) with a diagonal matrix of space-time basis function $\mathbf{N}_{xti}$ (this has the basis function N_{xti} along its main diagonal), integrating over a single element V_E and applying integration by parts results in:

$$\int_{V_E}\mathbf{N}_{xti}\mathbf{r}dV_{xt}-\int_{\Gamma_E}\mathbf{N}_{xti}(\mathbf{n}_{xt}\cdot\mathbf{A}_{xt})^-(\Psi-\Psi_{bc})d\Gamma_{xt} \tag{95}$$

$$+\int_{V_E}(\nabla^2_{xt}\mathbf{N}_{xti})\mathbf{B}^*_{xt}\mathbf{P}^*_{xt}\mathbf{r}dV_{xt} \tag{96}$$

$$+\int_{\Gamma_E}\mathbf{n}_{xt}\cdot(\mathbf{N}_{xti}\nabla_{xt}(\mathbf{B}^*_{xt}\mathbf{P}^*_{xt}\mathbf{r})-(\nabla_{xt}\mathbf{N}_{xti})\mathbf{B}^*_{xt}\mathbf{P}^*_{xt}\mathbf{r})\,d\Gamma_{xt}=\mathbf{0}, \tag{97}$$

with a finite element expansion $\Psi=\sum_{j=1}^{\mathcal{N}}\mathbf{N}_{xtj}\mathbf{\Psi}_j$ (where $\mathbf{\Psi}_j$ is the order

$\mathcal{M}$ vector of unknowns at node j) and $\mathbf{r} = \mathbf{A}_{xt} \cdot \nabla_{xt}\Psi + \mathbf{H}\Psi - \mathbf{s}$. Using the eigen-decomposition $\mathbf{n}_{xt} \cdot \mathbf{A}_{xt} = \mathbf{L}_{xt}\mathbf{\Lambda}_{xt}\mathbf{R}_{xt}$ then $(\mathbf{n}_{xt} \cdot \mathbf{A}_{xt})^- = \mathbf{L}_{xt}\mathbf{\Lambda}^-_{xt}\mathbf{R}_{xt}$ with $\mathbf{\Lambda}^-_{xtkk} = \min\{0, \mathbf{\Lambda}_{xtkk}\}$. This eigen decomposition enables the boundary condition to be applied to incoming information only. We apply a zero boundary condition on every element that results in the term (97) being zero which results in:

$$\int_{V_E} \mathbf{N}_{xti}\mathbf{r}dV_{xt} - \int_{\Gamma_E} \mathbf{N}_{xti}(\mathbf{n}_{xt} \cdot \mathbf{A}_{xt})^-(\Psi - \Psi_{bc})d\Gamma_{xt} \tag{98}$$

$$+ \int_{V_E} (\nabla^2_{xt}\mathbf{N}_{xti})\mathbf{B}^*_{xt}\mathbf{P}^*_{xt}\mathbf{r}dV_{xt} = \mathbf{0}. \tag{99}$$

$\mathbf{P}^*_{xt}$ is defined, as previously, as a function of $\mathbf{A}^*_{xt}$ and the size and shape of the elements.

In the above we can work with the stabilization in diffusion form with (obtained from equation (94)):

$$\int_{V_E} \mathbf{N}_{xti}\mathbf{r}dV_{xt} - \int_{\Gamma_E} \mathbf{N}_{xti}(\mathbf{n}_{xt} \cdot \mathbf{A}_{xt})^-(\Psi - \Psi_{bc})d\Gamma_{xt} \tag{100}$$

$$+ \int_{V_E} (\nabla^2_{xt}\mathbf{N}_{xti})\mathbf{K}_{4h}(\nabla^2_{xt}\Psi)dV_{xt} = \mathbf{0}, \tag{101}$$

in which the $\mathcal{M} \times \mathcal{M}$ diagonal matrix containing the diffusion coefficients is:

$$\mathbf{K}_{4h} = \mathbf{B}^{*T}_{xt}\mathbf{P}^*_{xt}\mathbf{B}^*_{xt}, \tag{102}$$

or simplifying:

$$\mathbf{K}_{4h} = \mathbf{V}(\mathbf{A}_{xt} \cdot \nabla_{xt}\Psi)\mathbf{P}^*_{xt}\mathbf{V}(||\nabla^2_{xt}\Psi||^2_2)^{-1}\mathbf{V}(\mathbf{A}_{xt} \cdot \nabla_{xt}\Psi). \tag{103}$$

The resulting matrix $\mathbf{K}_{4h}$ is diagonal. One can also work with the residual only, by replacing $\mathbf{A}_{xt} \cdot \nabla_{xt}\Psi$ with the residual $\mathbf{r}$, which results in:

$$\mathbf{K}_{4h} = \mathbf{V}(\mathbf{r})^T\mathbf{P}^*_{xt}\mathbf{V}(||\nabla^2_{xt}\Psi||^2_2)^{-1}\mathbf{V}(\mathbf{r}), \tag{104}$$

which is always positive because $\mathbf{P}^*_{xt}$ is positive semi-definite (as well as diagonal) and in which $\mathbf{V}(\mathbf{r})$ is the diagonal matrix containing the residual of the governing equations on its diagonal. In this case the analysis shows

that:

$$\mathbf{B}^*_{xt} = \mathbf{V}(\mathbf{r})\mathbf{V}(||\nabla^2_{xt}\Psi||^2_2)^{-1}\mathbf{V}(\nabla^2_{xt}\Psi), \tag{105}$$

in the equations above.

5. Petrov-Galerkin - sixth order dissipation

Here we combine the fourth order and second order forms to form the sixth order form which is suitable for cubic polynomial elements or above.

For coupled equations the projection of $\mathbf{A}_{xt}$ onto $\nabla_{xt}\Psi$ may be written:

$$\mathbf{A}^*_{xt} = \mathbf{V}(\mathbf{A}_{xt}\cdot\nabla_{xt}\Psi)\mathbf{V}(||(\nabla_{xt}(\nabla^2_{xt}\Psi))||^2_2)^{-1}\nabla_{xt}(\nabla^2_{xt}\Psi). \tag{106}$$

Thus,

$$\mathbf{A}^*_{xt}\cdot\nabla_{xt}(\nabla^2_{xt}\Psi) = \mathbf{A}_{xt}\cdot\nabla_{xt}\Psi \tag{107}$$

or

$$\left(\mathbf{V}(\mathbf{A}_{xt}\cdot\nabla_{xt}\Psi)\mathbf{V}(||(\nabla_{xt}(\nabla^2_{xt}\Psi))||^2_2)^{-1}\nabla_{xt}(\nabla^2_{xt}\Psi)\right)\cdot\nabla_{xt}(\nabla^2_{xt}\Psi) = \mathbf{A}_{xt}\cdot\nabla_{xt}\Psi. \tag{108}$$

Since $\mathbf{A}^*_{xt}\cdot\nabla_{xt}\Psi + \mathbf{H}\Psi - \mathbf{s} = 0$ are a set of $\mathcal{M}$ independent scalar equations in which the μ^{th} scalar equation is:

$$a^*_{t\,\mu}\frac{\partial\Psi_\mu}{\partial t} + a^*_{x\mu}\frac{\partial\Psi_\mu}{\partial x} + a^*_{y_\mu}\frac{\partial\Psi_\mu}{\partial y} + a^*_{z\mu}\frac{\partial\Psi_\mu}{\partial z} + \sigma_\mu\Psi_\mu = \mathbf{s}_\mu \tag{109}$$

and $a^*_{t\,\mu} = \mathbf{A}^*_{t\,\mu\mu}$, $a^*_{x\mu} = \mathbf{A}^*_{x\mu\mu}$, $a^*_{y_\mu} = \mathbf{A}^*_{y_{\mu\mu}}$, $a^*_{z\mu} = \mathbf{A}^*_{z\mu\mu}$, $\sigma_\mu = \mathbf{H}_{\mu\mu}$ and Ψ_μ is the μ^{th} scalar in the vector Ψ. In equation (109) it is assumed that $\mathbf{H}$ is a diagonal. If it is not then the system of equations can be easily manipulated so as to diagonalise $\mathbf{H}$, see equations (45), (46), (47), (48). Since the equations have been uncoupled then the scalar equation methods described in the previous section can now be applied. This is effectively done below.

The sixth order Petrov-Galerkin's modified form of the differential equation is:

$$(\mathbf{I} - \nabla^2_{xt}(\nabla_{xt}\cdot\mathbf{A}^*_{xt})^T\mathbf{P}^*_{xt})(\mathbf{A}_{xt}\cdot\nabla_{xt}\Psi + \mathbf{H}\Psi - \mathbf{s}) = \mathbf{0}, \tag{110}$$

or equaivelently using equation (107):

$$(\mathbf{I} - \nabla^2_{xt}(\nabla_{xt} \cdot \mathbf{A}^*_{xt})^T \mathbf{P}^*_{xt})(\mathbf{A}^*_{xt} \cdot \nabla_{xt}(\nabla^2_{xt}\Psi) + \mathbf{H}\Psi - \mathbf{s}) = \mathbf{0}. \tag{111}$$

Testing equation (32) with a diagonal matrix of space-time basis function $\mathbf{N}_{xti}$ (this has the basis function N_{xti} along its main diagonal), integrating over a single element V_E and applying integration by parts results in:

$$\int_{V_E} \mathbf{N}_{xti}\mathbf{r}dV_{xt} - \int_{\Gamma_E} \mathbf{N}_{xti}(\mathbf{n}_{xt} \cdot \mathbf{A}_{xt})^-(\Psi - \Psi_{bc})d\Gamma_{xt} \tag{112}$$

$$+ \int_{V_E} ((\nabla_{xt}(\nabla^2_{xt}\mathbf{N}_{xti})) \cdot \mathbf{A}^*_{xt})^T \mathbf{P}^*_{xt}\mathbf{r}dV_{xt} = \mathbf{0}, \tag{113}$$

with a finite element expansion $\Psi = \sum_{j=1}^{\mathcal{N}} \mathbf{N}_{xtj}\mathbf{\Psi}_j$ (where $\mathbf{\Psi}_j$ is the order $\mathcal{M}$ vector of unknowns at node j) and $\mathbf{r} = \mathbf{A}_{xt} \cdot \nabla_{xt}\Psi + \mathbf{H}\Psi - \mathbf{s}$. We have set the surface integral to zero around each element which becomes part of the boundary conditions.

In the above we can work with the stabilization in diffusion form with:

$$\int_{V_E} \mathbf{N}_{xti}\mathbf{r}dV_{xt} - \int_{\Gamma_E} \mathbf{N}_{xti}(\mathbf{n}_{xt} \cdot \mathbf{A}_{xt})^-(\Psi - \Psi_{bc})d\Gamma_{xt} \tag{114}$$

$$+ \int_{V_E} (\nabla_{xt}(\nabla^2_{xt}\mathbf{N}_{xti}))^T \mathbf{K}_{6h}(\nabla_{xt}(\nabla^2_{xt}\Psi))dV_{xt} = \mathbf{0} \tag{115}$$

in which the $\mathcal{M} \times \mathcal{M}$ diagonal matrix containing the diffusion coefficients is:

$$\mathbf{K}_{6h} = \mathbf{V}(\mathbf{A}_{xt} \cdot \nabla_{xt}\Psi)\mathbf{P}^*_{xt}\mathbf{V}(||(\nabla_{xt}(\nabla^2_{xt}\Psi))||^2_2)^{-1}\mathbf{V}(\mathbf{A}_{xt} \cdot \nabla_{xt}\Psi). \tag{116}$$

The resulting matrix $\mathbf{K}_{6h}$ is diagonal. One can also work with the residual only, by replacing $\mathbf{A}_{xt} \cdot \nabla_{xt}\Psi$ with the residual $\mathbf{r}$, which results in:

$$\mathbf{K}_{6h} = \mathbf{V}(\mathbf{r})^T \mathbf{P}^*_{xt}\mathbf{V}(||\nabla_{xt}(\nabla^2_{xt}\Psi)||^2_2)^{-1}\mathbf{V}(\mathbf{r}) \tag{117}$$

which is always positive because $\mathbf{P}^*_{xt}$ is positive semi-definite (as well as diagonal) and in which $\mathbf{V}(\mathbf{r})$ is the diagonal matrix containing the residual of the governing equations on its diagonal. In this case the analysis shows

that:

$$\mathbf{A}^*_{xt} = \mathbf{V}(\mathbf{r})\mathbf{V}(||(\nabla_{xt}(\nabla^2_{xt}\Psi))||^2_2)^{-1}\nabla_{xt}(\nabla^2_{xt}\Psi), \tag{118}$$

in the equations above.

6. Petrov-Galerkin - eighth order dissipation

This dissipation can be used for quintic polynomials and above. The discretization becomes, following the albegra above:

$$\int_{V_E} \mathbf{N}_{xti}\mathbf{r}dV_{xt} - \int_{\Gamma_E} \mathbf{N}_{xti}(\mathbf{n}_{xt}\cdot\mathbf{A}_{xt})^-(\Psi-\Psi_{bc})d\Gamma_{xt} \tag{119}$$

$$+\int_{V_E} (\nabla^2_{xt}\nabla^2_{xt}\mathbf{N}_{xti})^T\mathbf{K}_{8h}(\nabla^2_{xt}\nabla^2_{xt}\Psi)dV_{xt} = \mathbf{0} \tag{120}$$

in which the $\mathcal{M}\times\mathcal{M}$ diagonal matrix containing the diffusion coefficients is:

$$\mathbf{K}_{8h} = \mathbf{V}(\mathbf{r})^T\mathbf{P}^*_{xt}\mathbf{V}((\nabla^2_{xt}\nabla^2_{xt}\Psi)^2)^{-1}\mathbf{V}(\mathbf{r}). \tag{121}$$

7. Petrov-Galerkin - tenth order dissipation

This dissipation can be used for fifth order polynomials and above. The discretization becomes, following the albegra above:

$$\int_{V_E} \mathbf{N}_{xti}\mathbf{r}dV_{xt} - \int_{\Gamma_E} \mathbf{N}_{xti}(\mathbf{n}_{xt}\cdot\mathbf{A}_{xt})^-(\Psi-\Psi_{bc})d\Gamma_{xt} \tag{122}$$

$$+\int_{V_E} (\nabla_{xt}(\nabla^2_{xt}\nabla^2_{xt}\mathbf{N}_{xti}))^T\mathbf{K}_{10h}(\nabla_{xt}(\nabla^2_{xt}\nabla^2_{xt}\Psi))dV_{xt} = \mathbf{0} \tag{123}$$

in which the $\mathcal{M}\times\mathcal{M}$ diagonal matrix containing the diffusion coefficients is:

$$\mathbf{K}_{10h} = \mathbf{V}(\mathbf{r})^T\mathbf{P}^*_{xt}\mathbf{V}(||\nabla_{xt}(\nabla^2_{xt}\nabla^2_{xt}\Psi)||^2_2)^{-1}\mathbf{V}(\mathbf{r}). \tag{124}$$

8. Petrov-Galerkin - combined order dissipation and efficient implementation using local coordinates

Combining dissipation one may apply the approach with different polynomials in different coordinates say. The result is:

$$\int_{V_E} \mathbf{N}_{xti} \mathbf{r} dV_{xt} - \int_{\Gamma_E} \mathbf{N}_{xti} (\mathbf{n}_{xt} \cdot \mathbf{A}_{xt})^- (\Psi - \Psi_{bc}) d\Gamma_{xt} \tag{125}$$

$$+ \int_{V_E} (\ (\nabla_{xt} \mathbf{N}_{xti})^T \mathbf{K}_{2h} (\nabla_{xt} \Psi) + (\nabla^2_{xt} \mathbf{N}_{xti}) \mathbf{K}_{4h} (\nabla^2_{xt} \Psi) \tag{126}$$

$$+ (\nabla_{xt} \nabla^2_{xt} \mathbf{N}_{xti})^T \mathbf{K}_{6h} (\nabla_{xt} \nabla^2_{xt} \Psi) \tag{127}$$

$$+ (\nabla^2_{xt} \nabla^2_{xt} \mathbf{N}_{xti}) \mathbf{K}_{8h} (\nabla^2_{xt} \nabla^2_{xt} \Psi) \ ) dV_{xt} = \mathbf{0}. \tag{128}$$

In addition, in order to make the implementations more efficient it can be appropriate to form the derivatives using local coordinates. To this end we suggest replacing

$$\nabla^2_{xt} \Psi \tag{129}$$

in ALL the above equations with

$$\nabla^2_{\xi\tau} \Psi \tag{130}$$

in which ξ and τ are the local coordinates in space and in time, respectively, of the FEM or Spectral element approach. Equation (134) then becomes:

$$\int_{V_E} \mathbf{N}_{xti} \mathbf{r} dV_{xt} - \int_{\Gamma_E} \mathbf{N}_{xti} (\mathbf{n}_{xt} \cdot \mathbf{A}_{xt})^- (\Psi - \Psi_{bc}) d\Gamma_{xt} \tag{131}$$

$$+ \int_{V_E} (\ (\nabla_{xt} \mathbf{N}_{xti})^T \mathbf{K}_{2h} (\nabla_{xt} \Psi) + (\nabla^2_{\xi\tau} \mathbf{N}_{xti}) \mathbf{K}_{4h} (\nabla^2_{\xi\tau} \Psi) \tag{132}$$

$$+ (\nabla_{xt} \nabla^2_{\xi\tau} \mathbf{N}_{xti})^T \mathbf{K}_{6h} (\nabla_{xt} \nabla^2_{\xi\tau} \Psi) \tag{133}$$

$$+ (\nabla^2_{\xi\tau} \nabla^2_{\xi\tau} \mathbf{N}_{xti}) \mathbf{K}_{8h} (\nabla^2_{\xi\tau} \nabla^2_{\xi\tau} \Psi) \ ) dV_{xt} = \mathbf{0}. \tag{134}$$

9. Specifics for LBB stability of the Navier-Stokes equations

The Navier-Stokes equations often requires the use of a mixed formulation in order to achieve stability of the discretized Navier-Stokes equations and avoid checkerboard and possibly other pressure modes. This typically takes the form of using a polynomial of degree one less than for velocity. This

however, complicates the numerical method and thus one may instead choose to use numerical dissipation of pressure to achieve the same goal. That is introduce say a 2nd, 4th or 6th order dissipation term in pressure. If the magnitude of this is large enough this will reduce the polynomial order by one say if we use a 6th order dissipation term - similar to above - with a 3rd order polynomial in each element. This will reduce the polynomial to quadratic if the magnitude of the dissipation is large enough. In addition, introducing dissipation in pressure also allows the flexibility to use a minimal quantity of dissipation that achieves the required stability and thus improves accuracy.

It remains to be seen if the above can be relied on to perform adequate dissipation to remove the pressure mode(s). However, the current assumption is that its not. Also the dissipation of velocity acts to reduce the effectiveness (in terms of LBB stability) of any dissipation we introduce for pressure. One method to deal with this is to introduce the same or more (taking into account the dimensions difference of the continuity and momentum equations) dissipation in pressure as used for velocity. Another approach is to always add a certain amount of dissipation for pressure to, hopefully, achieve LBB stability.

Suppose each of the velocity components dissipation are given by equation (116) then once these are applied one can adjust the dissipation for pressure from their values

$$\mathbf{K}_{6hx} = \mathbf{V}(\mathbf{r})\mathbf{G}_x^*\mathbf{V}(||(\nabla_x(\nabla_x^2\Psi))||_2^2)^{-1}\mathbf{V}(\mathbf{r}), \tag{135}$$

in which $\mathbf{G}_x^*$ is:

$$\mathbf{G}_x^* = \frac{1}{4}(||\mathbf{J}_x^{-1}||_2)^{-1}. \tag{136}$$

The final pressure matrix dissipation may be obtained from:

$$\mathbf{K}_{6p} = \left(\mathbf{K}_{6hx1}^2 + \mathbf{K}_{6hx2}^2 + \mathbf{K}_{6hx3}^2\right)^{\frac{1}{2}}, \tag{137}$$

in which $\mathbf{K}_{6hx1}$ is the dissipation from equation (136) associated with the x-coordinate and $\mathbf{K}_{6hx2}$ the y-coordinate and $\mathbf{K}_{6hx3}$ the z-coordinate. The reason why we use $\mathbf{G}_x^*$ above rather than $\mathbf{P}_x^*$ is to take into account the dimensionality difference between the momentum and continuity equations. One should add this dissipation to pressure along with the previous dissipation

that aims to reduce numerical oscillations.

Alternatively, as discussed one may also choose to use a dissipation for pressure based on reducing the polynomial order and dimensional arguments so that it becomes:

$$\mathbf{K}_{6p} = \frac{1}{4}(||\mathbf{J}_x^{-1}\mathbf{u}||_2)^{-1}(||\mathbf{J}_x^{-1}||_2^4)^{-1}. \tag{138}$$

The resulting 6th order dissipation term is:

$$\int_{V_E} (\nabla_x(\nabla_x^2\mathbf{N}_{xti}))^T\mathbf{K}_{6p}(\nabla_x(\nabla_x^2\Psi))dV_{xt}, \tag{139}$$

which acts only in Cartesian space even though the integration is over space-time.

Equations (138) and (139) are amended when using derivatives of local coordinates too:

$$\mathbf{K}_{6p} = \frac{1}{4}(||\mathbf{J}_x^{-1}\mathbf{u}||_2)^{-1}. \tag{140}$$

The resulting 6th order dissipation term is:

$$\int_{V_E} (\nabla_x(\nabla_\xi^2\mathbf{N}_{xti}))^T\mathbf{K}_{6p}(\nabla_x(\nabla_\xi^2\Psi))dV_{xt}. \tag{141}$$

10. Discretization of the incompressible continuity equation and pressure term in the momentum equations

The continuity equation:

$$\nabla_x\mathbf{u} = 0, \tag{142}$$

can be discretized by either integrating by parts twice and addining in the pressure stabilization terms for LBB stability and for numerical oscillations:

$$\int_{V_E} \mathbf{N}_{xti}\nabla_x\cdot\mathbf{u}dV_{xt} + \int_{\Gamma_E} \mathbf{N}_{xti}\mathbf{n}_x\cdot\frac{1}{2}(\mathbf{u}-\mathbf{u}_{bc})d\Gamma_x \tag{143}$$

$$+\int_{V_E} \nabla_x(\nabla_x^2\mathbf{N}_{xti})(\mathbf{K}_{6p}+\mathbf{K}_{6h})\nabla_x(\nabla_x^2 p)dV_{xt} = 0, \tag{144}$$

in which $\mathbf{u}_{bc}$ is the velocity just inside the neighboring element to element E, or by integrating by part once in order to achieve the coupling between the elements:

$$-\int_{V_E}(\nabla_x \mathbf{N}_{xti})\cdot\mathbf{u}dV_{xt}+\int_{\Gamma_E}\mathbf{N}_{xti}\mathbf{n}_x\cdot\frac{1}{2}(\mathbf{u}+\mathbf{u}_{bc})d\Gamma_x \tag{145}$$

$$+\int_{V_E}\nabla_x(\nabla_x^2\mathbf{N}_{xti})(\mathbf{K}_{6p}+\mathbf{K}_{6h})\nabla_x(\nabla_x^2 p)dV_{xt}=0. \tag{146}$$

For the discretization of grad, ∇, used in the discretization of pressure p in the momentum equations we use the transpose of the resulting matrix from (145).

For compressible flow the governing equation is:

$$\frac{\partial\rho}{\partial t}+\nabla_x\cdot\rho\mathbf{u}=0, \tag{147}$$

and the discretization becomes:

$$\int_{V_E}\left(\mathbf{N}_{xti}\frac{\partial\rho}{\partial t}-(\nabla_x\mathbf{N}_{xti})\cdot\rho\mathbf{u}\right)dV_{xt} \tag{148}$$

$$+\int_{\Gamma_E}\mathbf{N}_{xti}\mathbf{n}_x\cdot\frac{1}{2}(\rho\mathbf{u}+\rho_{bc}\mathbf{u}_{bc})d\Gamma_x \tag{149}$$

$$+\int_{V_E}(\nabla_x(\nabla_x^2\mathbf{N}_{xti}))\mathbf{K}_{6p}(\nabla_x(\nabla_x^2 p))dV_{xt} \tag{150}$$

$$+\int_{V_E}(\nabla_{xt}(\nabla_{xt}^2\mathbf{N}_{xti}))\mathbf{K}_{6h}(\nabla_{xt}(\nabla_{xt}^2 p))dV_{xt}=0. \tag{151}$$

As an alternative to using a simple average of the mass flux between elements, that is $\frac{1}{2}(\rho\mathbf{u}+\rho_{bc}\mathbf{u}_{bc})$, one may decide to use a Harmonic average weighted using the volume of the neighboring elements:

$$\frac{\frac{1}{\mathcal{V}_{bc}}\rho\mathbf{u}+\frac{1}{\mathcal{V}_e}\rho_{bc}\mathbf{u}_{bc}}{\frac{1}{\mathcal{V}_{bc}}+\frac{1}{\mathcal{V}_e}}, \tag{152}$$

or possibly:

$$\frac{\frac{1}{\mathcal{V}_{bc}\rho_{bc}}\rho\mathbf{u} + \frac{1}{\mathcal{V}_e\rho}\rho_{bc}\mathbf{u}_{bc}}{\frac{1}{\mathcal{V}_{bc}\rho_{bc}} + \frac{1}{\mathcal{V}_e\rho}}, \tag{153}$$

in which $\mathcal{V}_e$ is the volume of the current finite element E and $\mathcal{V}_{bc}$ is the volume of the neighboring element.

11. The non-conservative form thats conservative

The conservative form of the transport equation for field Ψ is:

$$\frac{\partial\Psi}{\partial t} + \nabla_x \cdot \mathbf{u}\Psi = s, \tag{154}$$

and non-conservative form:

$$\frac{\partial\Psi}{\partial t} + \mathbf{u} \cdot \nabla_x\Psi = s. \tag{155}$$

Assuming for the time being divergence free, $\nabla_x \cdot \mathbf{u} = 0$, incompressible flow then the difference between the two forms is that the conservative form has small sinks and sources from the non-divergence behavior (at the discrete level) of the flow locally and the non-conservative form is non-conservative when the basis functions of Ψ are not the test functions of the continuity equation or a stabilization term in pressure is added to the continuity equation. These disadvantages can be eliminated by expanding the conservative form:

$$\frac{\partial\Psi}{\partial t} + \mathbf{u} \cdot \nabla_x\Psi + \Psi\nabla_x \cdot \mathbf{u} = s, \tag{156}$$

and then replacing $\nabla_x \cdot \mathbf{u}$ with the continuity equation so the term $\Psi\nabla_x \cdot \mathbf{u}$ discretized becomes for 6th order dissipation:

$$\int_{V_E} \mathbf{N}_{xti}\Psi\nabla_x\cdot\mathbf{u}dV_{xt} + \int_{\Gamma_E}\Psi\mathbf{N}_{xti}\mathbf{n}_x\cdot\frac{1}{2}(\mathbf{u}-\mathbf{u}_{bc})d\Gamma_x \tag{157}$$

$$+\int_{V_E}\Psi(\nabla_x(\nabla_x^2\mathbf{N}_{xti}))\mathbf{K}_{6p}(\nabla_x(\nabla_x^2 p))dV_{xt}. \tag{158}$$

Thus, the discretization of (154) is:

$$\int_{V_E}\mathbf{N}_{xti}\left(\frac{\partial\Psi}{\partial t}+\nabla_x\cdot\mathbf{u}\Psi-s\right)dV_{xt}+\int_{\Gamma_E}\mathbf{N}_{xti}\mathcal{S}(\mathbf{n}_x\cdot\mathbf{u})(\Psi-\Psi_{bc})d\Gamma_x \tag{159}$$

$$-\int_{V_E}\mathbf{N}_{xti}\Psi\nabla_x\mathbf{u}dV_{xt}-\int_{\Gamma_E}\frac{1}{2}\Psi\mathbf{N}_{xti}\mathbf{n}_x\cdot(\mathbf{u}-\mathbf{u}_{bc})d\Gamma_x \tag{160}$$

$$-\int_{V_E}\Psi(\nabla_x(\nabla_x^2\mathbf{N}_{xti}))\mathbf{K}_{6p}(\nabla_x(\nabla_x^2 p))dV_{xt} \tag{161}$$

$$+\int_{V_E}(\nabla_{xt}(\nabla_{xt}^2\mathbf{N}_{xti}))\mathbf{K}_{6h}(\nabla_{xt}(\nabla_{xt}^2\Psi))dV_{xt}, \tag{162}$$

in which $\mathcal{S}(a)=a$ if $a>0$ else $\mathcal{S}(a)=0$. Notice that this also includes the stabilization term (162) which attempts to reduce Gibbs oscillations.

12. Solving coupled equations with alternating point and transport problems

Often one needs to solve for complex thermodynamics or chemistry at a point because thats what the current codes do. However, one can superimpose the transport methods above onto this as follows.

Suppose the equations to be solved at a point are:

$$\frac{\hat{\Psi}^{n+1}-\hat{\Psi}^n}{\Delta t_{pt}}=s_{pt}(\hat{\Psi}^{n+1},\hat{\Psi}^n), \tag{163}$$

to obtain $\hat{\Psi}^{n+1}$, then typically the solver returns back $\hat{\Psi}^{n+1}$ only and thus we need to determine the source for the transport equation, s_a, from:

$$s_a = \frac{\hat{\Psi}^{n+1} - \hat{\Psi}^n}{\Delta t_{pt}}. \tag{164}$$

Now this is the source for the complex coupled process and can be placed into a transport equation, for example:

$$\frac{\Psi^{n+1} - \Psi^n}{\Delta t} + \mathbf{u} \cdot \nabla_x \Psi = s_a, \tag{165}$$

to obtain Ψ^{n+1}, then rearranging this equation the transport terms can be represented by the source and time terms:

$$-\mathbf{u} \cdot \nabla_x \Psi = s_c, \tag{166}$$

with, from equation (165):

$$s_c = \frac{\Psi^{n+1} - \Psi^n}{\Delta t} - s_a. \tag{167}$$

The point problem can be solved once again with an improved, transport corrected, source:

$$\frac{\hat{\Psi}^{n+1} - \hat{\Psi}^n}{\Delta t_{pt}} = s_{pt}(\hat{\Psi}^{n+1}, \hat{\Psi}^n) + s_c, \tag{168}$$

then

$$s_a = \frac{\hat{\Psi}^{n+1} - \hat{\Psi}^n}{\Delta t_{pt}} - s_c, \tag{169}$$

which is placed in equation (165) and so on until convergence.

However, this approach needs the introduction of basis functions in time when using the space-time approach for both s_a and s_c. This is achieved as follows. Suppose:

$$\Delta t = \mathcal{N}_t \Delta t_{pt}, \tag{170}$$

for some integer $\mathcal{N}_t$. Suppose the FEM basis functions in time are N_{tj} and

thus

$$s_a = \sum_j N_{tj} s_{aj}, \tag{171}$$

and

$$s_c = \sum_j N_{tj} s_{cj}. \tag{172}$$

To achieve this equation (169) is projected onto the basis functions N_{tj} to form s_a using a Galerkin projection. Similarly s_c is projected onto the same basis functions N_{tj} using equation (167).

13. DG discretization of diffusion and viscous terms

Here we outline our approach to discretizing the second order terms involving conductivity/diffusivity and viscous terms. The approach produces a compact stencil - the coupling is only between elements that share a face with the current element - and is accurate. Its main disadvantage is that it does not result in a symmetric-positive-definite matrix for the second order terms. However, this is not a major disadvantage as typically we solve systems involving advection which results in non-symmetry of the matrices obtained. The basic idea of the approach is to integrate the second order terms by parts resulting in a first order term on the surface integral between the elements. This first order term is then the subject to a further approximation by integrating across both elements associated with a surface.

13.1. DG discretization of viscosity in stress form

In tensor form the viscosity discretization proceeds as described in the previous section, but for each velocity component u, v and w separately (or u_1, u_2, u_3). For the stress form of viscosity, consider the momentum equation:

$$\rho \frac{Du_i}{Dt} = \frac{\partial \sigma_{i\,k}}{\partial x_k} + s_{mom} \tag{173}$$

with

$$\sigma_{i\,k} = \mu_{i\,k} \left(\frac{\partial u_k}{\partial x_i} + \frac{\partial u_i}{\partial x_k} - \delta_{i\,k} \frac{2}{3} \nabla \cdot \mathbf{u} \right) + \mu_{vol} \delta_{i\,k} \nabla \cdot \mathbf{u}. \tag{174}$$

in which μ_{vol} is the volumetric viscosity.
The viscous term expanded becomes:

$$\frac{\partial(\mu_{xx}(\frac{\partial u}{\partial x}+\frac{\partial u}{\partial x})-(\frac{2}{3}\mu_{xx}-\mu_{vol})(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}))}{\partial x}+\frac{\partial \mu_{xy}(\frac{\partial v}{\partial x}+\frac{\partial u}{\partial y})}{\partial y}+\frac{\partial \mu_{xz}(\frac{\partial w}{\partial x}+\frac{\partial u}{\partial z})}{\partial z}, \tag{175}$$

$$\frac{\partial \mu_{yx}(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x})}{\partial x}+\frac{\partial(\mu_{yy}(\frac{\partial v}{\partial y}+\frac{\partial v}{\partial y})-(\frac{2}{3}\mu_{yy}-\mu_{vol})(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}))}{\partial y}+\frac{\partial \mu_{yz}(\frac{\partial w}{\partial y}+\frac{\partial v}{\partial z}))}{\partial z}, \tag{176}$$

$$\frac{\partial \mu_{zx}(\frac{\partial u}{\partial z}+\frac{\partial w}{\partial x})}{\partial x}+\frac{\partial \mu_{zy}(\frac{\partial v}{\partial z}+\frac{\partial w}{\partial y})}{\partial y}+\frac{\partial(\mu_{zz}(\frac{\partial w}{\partial z}+\frac{\partial w}{\partial z})-(\frac{2}{3}\mu_{zz}-\mu_{vol})(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}))}{\partial z}. \tag{177}$$

The DG discretization of these becomes for u:

$$\int_E \frac{\partial N_i}{\partial x}\left(2\mu_{xx}\frac{\partial u}{\partial x}-\left(\frac{2}{3}\mu_{xx}-\mu_{vol}\right)\nabla\cdot\mathbf{u}\right)+\frac{\partial N_i}{\partial y}\mu_{xy}\left(\frac{\partial v}{\partial x}+\frac{\partial u}{\partial y}\right)+\frac{\partial N_i}{\partial z}\mu_{xz}\left(\frac{\partial w}{\partial x}+\frac{\partial u}{\partial z}\right)dV+ \tag{178}$$

$$\int_{\Gamma_E} N_i\left(n_x\left(2\mu_{xx}\frac{\partial u}{\partial x}-\left(\frac{2}{3}\mu_{xx}-\mu_{vol}\right)\nabla\cdot\mathbf{u}\right)+n_y\mu_{xy}\left(\frac{\partial v}{\partial x}+\frac{\partial u}{\partial y}\right)+n_z\mu_{xz}\left(\frac{\partial w}{\partial x}+\frac{\partial u}{\partial z}\right)\right)d\Gamma, \tag{179}$$

for v:

$$\int_E \frac{\partial N_i}{\partial x}\mu_{yx}\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)+\frac{\partial N_i}{\partial y}\left(2\mu_{yy}\frac{\partial v}{\partial y}-\left(\frac{2}{3}\mu_{yy}-\mu_{vol}\right)\nabla\cdot\mathbf{u}\right)+\frac{\partial N_i}{\partial z}\mu_{yz}\left(\frac{\partial w}{\partial y}+\frac{\partial v}{\partial z}\right)dV+ \tag{180}$$

$$\int_{\Gamma_E} N_i\left(n_x\mu_{yx}\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)+n_y\left(2\mu_{yy}\frac{\partial v}{\partial y}-\left(\frac{2}{3}\mu_{yy}-\mu_{vol}\right)\nabla\cdot\mathbf{u}\right)+n_z\mu_{yz}\left(\frac{\partial w}{\partial y}+\frac{\partial v}{\partial z}\right)\right)d\Gamma, \tag{181}$$

for w:

$$\int_E \frac{\partial N_i}{\partial x}\mu_{zx}\left(\frac{\partial u}{\partial z}+\frac{\partial w}{\partial x}\right)+\frac{\partial N_i}{\partial y}\mu_{zy}\left(\frac{\partial v}{\partial z}+\frac{\partial w}{\partial y}\right)+\frac{\partial N_i}{\partial z}(\mu_{zz}2\frac{\partial w}{\partial z}-\left(\frac{2}{3}\mu_{zz}-\mu_{vol}\right)\nabla\cdot\mathbf{u}\Big)\,dV+ \tag{182}$$

$$\int_{\Gamma_E} N_i\left(n_x\mu_{zx}\left(\frac{\partial u}{\partial z}+\frac{\partial w}{\partial x}\right)+n_y\mu_{zy}\left(\frac{\partial v}{\partial z}+\frac{\partial w}{\partial y}\right)+n_z\left(\mu_{zz}2\frac{\partial w}{\partial z}-\left(\frac{2}{3}\mu_{zz}-\mu_{vol}\right)\nabla\cdot\mathbf{u}\right)\right)d\Gamma. \tag{183}$$

13.2. High order linear DG viscosity scheme

Here we describe the high order linear scheme. This forms the first order derivatives on the boundaries of the elements and as such has advantages over the, linear at least, interior penalty function method. Although its disadvantages are that it does not have a maximum principle like the interior penalty function method for linear elements and also results in non-symmetric matrices. It does however result in a compact stencil with an element coupling only to its surrounding elements. Its performance has been very impressive in terms of accuracy and has a null space that is not easily excited. The method has the same volume treatment as the interior penalty function method and differers only in the surface integral around each element in which the first order derivatives are evaluated. For example:

$$\int_E N_i\frac{\partial\mu\frac{\partial u}{\partial x}}{\partial x}dV=-\int_E\frac{\partial N_i}{\partial x}\mu\frac{\partial u}{\partial x}dV+\int_{\Gamma_E}N_in_x\mu\frac{\partial u}{\partial x}d\Gamma, \tag{184}$$

in order to evaluate the derivative $\frac{\partial u}{\partial x}$ on the boundary of the element Γ_E we integrate over the volume of two neighboring elements in order to calculate the derivative on the element face between the two elements using:

$$\int_{2E}N_i\frac{\partial u}{\partial x}dV-\frac{1}{2}\int_{\Gamma_{E1}}N_in_x(u-u_{bc})d\Gamma-\frac{1}{2}\int_{\Gamma_{E2}}N_in_x(u-u_{bc})d\Gamma, \tag{185}$$

in which Γ_{E1} is the the shared face but within element 1 and similarly Γ_{E2} is the the shared face but within element 2 and u_{bc} is the value of u in the

neighboring element along the face. Also

$$u_x = \sum_j N_j u_{xj} \approx \frac{\partial u}{\partial x}. \tag{186}$$

Then the derivative used within equation (184) is:

$$\frac{1}{2}\left(\frac{\partial u}{\partial x} + \frac{\partial u}{\partial x}|_{bc}\right). \tag{187}$$

13.3. Calculating the high order derivatives on element boundaries

In order to obtain the high order derivatives used in the calculation of the limited diffusion term, Eqn. (**??**), the finite element solution within each element is used along with boundary conditions from the finite element solution of the surrounding elements or the boundary conditions on the domain, if the elements are next to the domain boundaries. That is $\frac{\partial T^n}{\partial x}$ is calculated from

$$B\underline{T}^n_{fem_x} = \underline{v}^n_x, \quad B\underline{T}^n_{fem_y} = \underline{v}^n_y, \quad B\underline{T}^n_{fem_z} = \underline{v}^n_z, \tag{188}$$

with $B_{ij} = \int N_i N_j dV$, $T_{fem_x} = \sum_j N_j T_{fem_{xj}}$ and is discontinuous as the basis functions N_i are discontinuous between elements. In addition,

$$\begin{aligned}
\underline{v}^n_x &= \int N_i \frac{\partial T^n_{fem}}{\partial x} dV - \int_{\Gamma_{ele}} n_x N_i (T^n_{fem_{current}} - T^n_{fem_{nab}}) d\Gamma, \\
\underline{v}^n_y &= \int N_i \frac{\partial T^n_{fem}}{\partial y} dV - \int_{\Gamma_{ele}} n_y N_i (T^n_{fem_{current}} - T^n_{fem_{nab}}) d\Gamma, \\
\underline{v}^n_z &= \int N_i \frac{\partial T^n_{fem}}{\partial z} dV - \int_{\Gamma_{ele}} n_z N_i (T^n_{fem_{current}} - T^n_{fem_{nab}}) d\Gamma.
\end{aligned} \tag{189}$$

Dirichlet boundary conditions are applied through the surface integral around each element Γ_{ele}.

The values of the derivatives either side of the control volume face are placed into Eqn. (**??**). These may be the same value for example within an element or when there is continuity of solution T^n or T^n_{fem} between elements. The same approach is also used to form the diffusion operator for DG based on equation (**??**). The solution of equations (188) are local to each element as the matrix is a Discontinuous Galerkin mass matrix B and thus does not

couple the elements.

14. Solving the Linear Equations

One of the main advantages of the finite element high resolution method (HRFEM) that it shares with most other FEM methods, is that the equations involve diagonal dominant mass matrixes which are well conditioned and have a condition number independent of the grid size.

In contrast to first order discretization methods, the HRFEM equations have coupling in all directions. The HRFEM method used here is obtained by making each element a CV and using a mapping between the CV and the FEM solution. The FEM solution is then used as the high order flux along the CV faces. The HRFEM method requires the inverse of the consistent mass matrix in order to calculate incoming control volume fluxes accurately - this inverse is a full matrix. Thus, this coupling in practice can only be realized explicitly in the iterative scheme. The HRFEM method has been generalised with a bi-jective mapping between the FEM and CV solutions. The discontinuous HRFEM method also uses consistent mass matrices, but these are local to an element so they are more manageable and can be treated implicitly.

There are a number of options available for solving the non-linear HRFEM equations. One can linearize the global equation set, treating implicitly or explicitly the down stream element coupling (inclusion of down stream coupling may result in poorer conditioned matrices from the discretization). Then a global set of linear equations would be solved each non-linear iteration by for example using SSOR preconditioning for GMRES (**?**). Alternatively, one can sweep through each CV, resolving all the non-linear equations local to each CV with a suitable liberalization procedure.

The global or local to an element liberalization can be achieved using the Newton-Raphson method, although this has quadratic convergence properties it is prone to failure when there does not exist a good initial guess. The most robust method reported for other flux limiting methods is to linearize on the first-order equations (see **?**). This involves solving a matrix equation with a matrix obtained from the underlying first order spatial discretization and the deviation of the high order scheme from this, would be treated explicitly as a source term. This has the advantage that the resulting matrix is well conditioned and also the non-linear convergence to a solution is usually

monotonic, due to the dissipative characteristics of the first order scheme and is thus the approach adapted here.