ST*n*.1 Scalar Transport, GWS^h + θTS *for all n*

Conservation principle:

$$\mathrm{L}(q) = \frac{\partial q}{\partial t} + \mathbf{u}\cdot\nabla q - \frac{1}{\mathrm{Pa}}\nabla\cdot(1+\mathrm{Re}^t)\nabla q - s = 0$$

$$\ell(q) = \nabla q\cdot\hat{\mathbf{n}} + \mathrm{Pb}(q - q_{ref}) + f_n = 0$$

GWS^h + θTS ⇒ matrix statement:

$$[\mathrm{JAC}]\{\Delta Q\} = -\Delta t\{\mathrm{RES}\}_n,\ \{Q\}_{n+1} = \{Q\}_n + \{\Delta Q\}$$

$$[\mathrm{JAC}], \{\mathrm{RES}\} \Rightarrow \mathrm{S}_e\{\mathrm{WS}\}_e$$

$$[\mathrm{JAC}]_e = [\mathrm{MASS}]_e + \theta\Delta t\big([\mathrm{UVWVEL}]_e + [\mathrm{DIFF}]_e + [\mathrm{HBC}]_e\big)$$

$$\{\mathrm{RES}\}_e = [\mathrm{UVWEL} + \mathrm{DIFF} + \mathrm{HBC}]_e\{Q\}_e - \{\mathrm{b}(s, q_{ref}, f_n)\}$$

Asymptotic error estimate:

$$q(\mathbf{x},t) = q^h(\mathbf{x},t) + e^h(\mathbf{x},t)$$

$$\left\| e^h(t) \right\|_E \le \mathrm{C}h^{2\gamma}\left\|\mathrm{data}\right\|^2_{\mathrm{L}2} + \mathrm{C}_t\Delta t^{f(\theta)}\left\|q_0\right\|_E \quad, \gamma = \min(1; k, r-1 \text{ for } \mathrm{Pa}^{-1} > 0)$$

norm:

$$\left\|q^h(t)\right\|_E \equiv \frac{1}{2}\int_\Omega \mathrm{Pa}^{-1}\nabla q^h\cdot(1+\mathrm{Re}^t)\nabla q^h \mathrm{d}\tau + \frac{1}{2}\int_{\partial\Omega}\mathrm{Pb}(q^h)^2\mathrm{d}\sigma$$

$$= \frac{1}{2}\sum_e \{Q(n\Delta t)\}^T_e[\mathrm{DIFF} + \mathrm{HBC}]_e\{Q(n\Delta t)\}_e$$

STn.2 GWS^h + θTS ⇒ Newton template, *for all n*

Newton statement components

$$[\mathrm{JAC}]_e = [\mathrm{MASS}]_e + \theta\Delta t\left([\mathrm{UVWVEL}]_e + [\mathrm{DIFF}]_e + [\mathrm{HBC}]_e\right)$$

$$\Delta t\{\mathrm{RES}\}_e = \Delta t\left(([\mathrm{UVWVEL}]_e + [\mathrm{DIFF}]_e + [\mathrm{HBC}]_e)\{Q\}_n - \{\mathrm{b}\}_{n+\theta}\right)$$

Template pseudo-code, for *any* $\{N_k(\zeta, \eta)\}$, $1 \le K \le n$

$$\{\mathrm{WS}\}_e \equiv (\mathrm{const})(\mathrm{avg})_e\{\mathrm{dist}\}_e(\mathrm{metric})[\mathrm{Matrix}]\{Q \textit{ or } \mathrm{data}\}_e$$

$$\begin{aligned}[\mathrm{JAC}]_e = {} & (\ )(\ )\{\ \}(1)[\mathrm{M200}][\ ] + (\theta\Delta t)(\ )\{\mathbf{U}K\}(0)[\mathrm{M300}\,K]_e[\ ] \\ & + (\theta\Delta t, \mathrm{Pa}^{-1})(\ )\{1+\mathrm{Ret}\}(-1)[\mathrm{M30}\,KK]_e[\ ] \\ & + (\theta\Delta t, \mathrm{Pb}/\mathrm{Pa})(\ )\{1+\mathrm{Ret}\}(1)[\mathrm{N3000}][\ ]\end{aligned}$$

$$\begin{aligned}\Delta t\{\mathrm{RES}\}_e = {} & (\Delta t)(\ )\{\mathbf{U}K\}(0)[\mathrm{M300}\,K]\{\mathrm{QN}\} \\ & + (\Delta t, \mathrm{Pa}^{-1})(\ )\{1+\mathrm{Ret}\}(-1)[\mathrm{M30}\,KK]_e\{\mathrm{QN}\} \\ & + (\Delta t, \mathrm{Pb/Pa})(\ )\{1+\mathrm{Ret}\}(1)[\mathrm{N3000}]\{\mathrm{QN}\} \\ & + (-\Delta t)(\ )(\ )(1)[\mathrm{M200}]\{\mathrm{SRC}\} + (\Delta t)(\ )(\ )(1)[\mathrm{N200}]\{\mathrm{FN}\} \\ & + (-\Delta t, \mathrm{Pb/Pa})(\ )\{1+\mathrm{Ret}\}(1)[\mathrm{N3000}]\{\mathrm{QR}\}\end{aligned}$$

STn.3 Dispersion Error Mode Identification

From n = 1 Peclet & traveling wave experiments

for Pe modest, GWS^h + θTS solutions "OK" for Ω^h good enough
for Pe large, dominant error mode is mesh scale oscillations

Taylor series enables decisive error characterization

D*E*:

$$\mathrm{L}(q) = q_t + f_x - \mathrm{Pa}^{-1} q_{xx} = 0, \quad f = uq \quad for \;\; n = 1$$

TS:

$$q_{n+1} = q_n + \Delta t q_t + \frac{1}{2}\Delta t^2 q_{tt} + \frac{1}{6}\Delta t^3 q_{ttt} + \cdots$$

for Pa^{-1}<< ε:

$$q_t \cong -f_x$$

$$q_{tt} \cong -f_{xt} = -(f_q q_t)_x = (f_q f_q q_x)_x \Rightarrow \beta(u^2 q_x)_x$$

$$q_{ttt} \cong (u^2 q_x)_{xt} \Rightarrow \gamma(u^2 q_{xt})_x$$

Substitute into TS, take limit Δ*t* ⇒ ε > 0, yields modified D*E*

*m*D*E*:

$$\mathrm{L}^m(q) = \mathrm{L}(q) - \frac{\Delta t}{2}\frac{\partial}{\partial x}\left(\beta u^2 \frac{\partial q}{\partial x}\right) - \frac{\Delta t^2}{6}\frac{\partial}{\partial x}\left(\gamma u^2 \frac{\partial^2 q}{\partial t \partial x}\right) + \mathrm{TE}$$

STn.4 Dispersion Error Mode Characterization

$\mathbf{D}E \Rightarrow m\mathbf{D}E$:

mDE:

$$L^m(q) = \left[1 - \frac{\partial}{\partial x}\left(\frac{\gamma(\Delta t u)^2}{6}\frac{\partial}{\partial x}\right)\right]\frac{\partial q}{\partial t} + u\frac{\partial q}{\partial x} - \frac{\partial}{\partial x}\left[\left(\mathrm{Pa}^{-1} + \beta u^2\right)\frac{\partial q}{\partial x}\right] \cong 0$$

Modal analysis on GWS^h (L^m(q)) + θTS, ω = 2π/λ

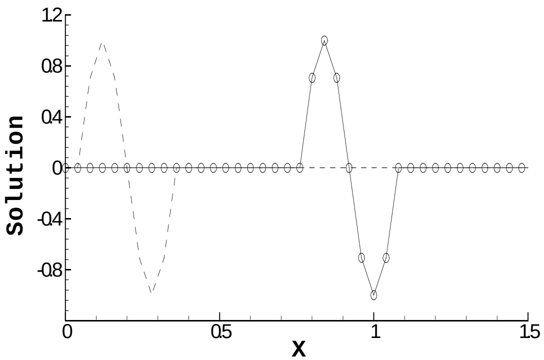
Fourier:

$$q(x,t) = \sum_{\omega} A_{\omega} q_{\omega}(x,t)$$

$$q_{\omega}(x,t) = \exp\left(\mathrm{i}\omega(x - ut)\right)$$

GWS^h:

$$q_{\omega}^{h}(j\Delta x, t) = \exp\left(\mathrm{i}\omega(j\Delta x - Ut)\right)$$



GWS^h + θTS:

$$Q_j(n\Delta t) = G q_{\omega}^{h}, \quad G = G_{\mathrm{real}} + \mathrm{i}G_{\mathrm{imag}}$$

$$G = f(\omega, \beta, \gamma, C, k, \theta)$$

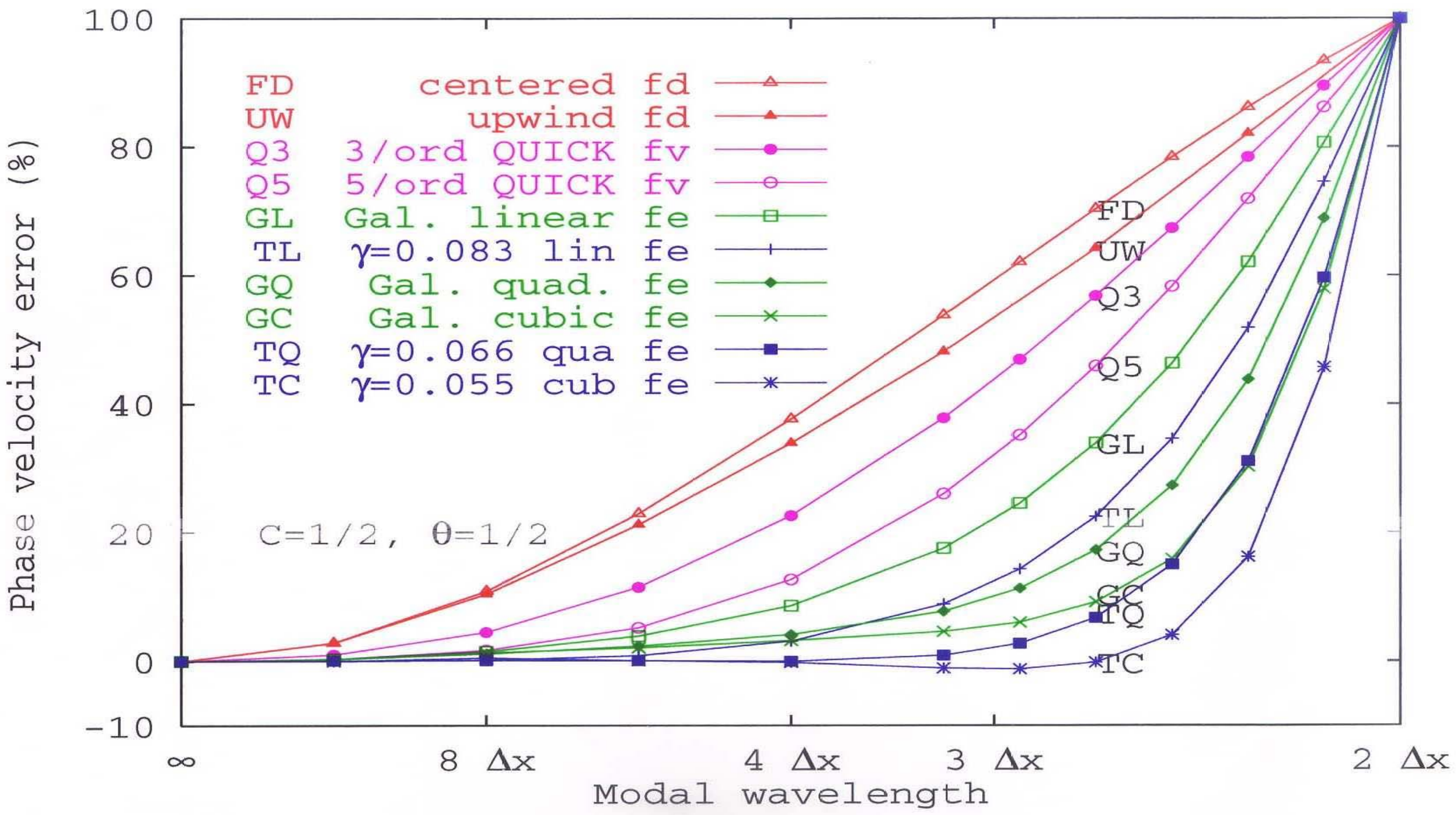
analysis:

$$\text{phase velocity}: U_{\omega} = \frac{1}{\omega\Delta x}\tan^{-1}[G_R / G_I]$$

$$\text{numerical diffusion}: |G| < 1$$

STn.5 Phase Velocity Error Spectra

Phase velocity U_ω *error* spectral distributions



STn.6 Traveling Wave, GWS^h (DE, mDE) + θTS

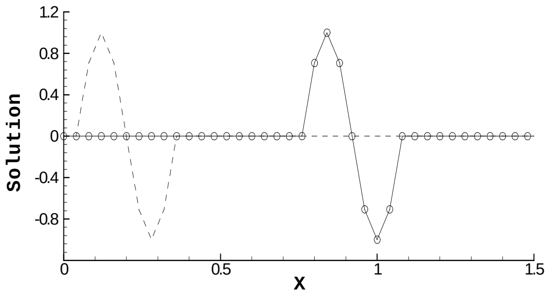
Problem statement

$$\mathrm{D}M : \mathrm{L}(q) = \frac{\partial q}{\partial t} + u\frac{\partial q}{\partial x} = 0$$

$$\mathrm{BC} : q(x = 0, t) = 0$$

$$\mathrm{IC} : q(x, t = t_0) = q_0(x)$$

Solution graph

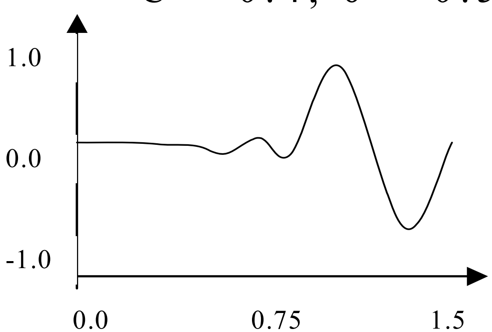


Characteristic solution

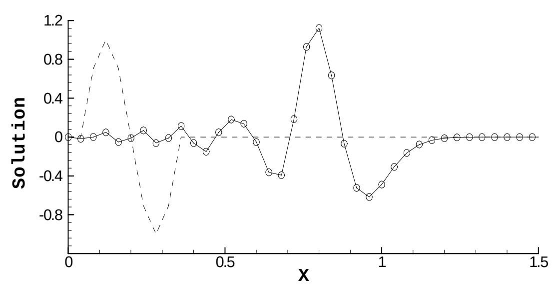
$$q(x,\ t) = q_0 \exp i(x - ut)$$

GWS^h on DE, mDE + θTS solutions, k = 1, C = $u\Delta t/\Delta x$

C = 0.4, θ = 0.5



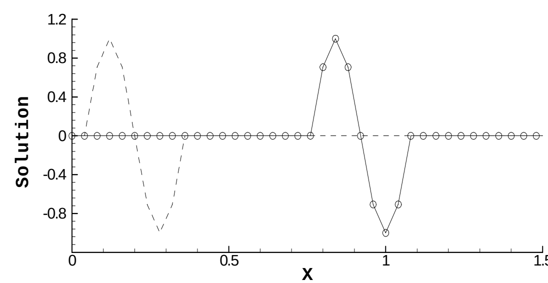
C = 1.0, θ = 0.5



C = 1.0

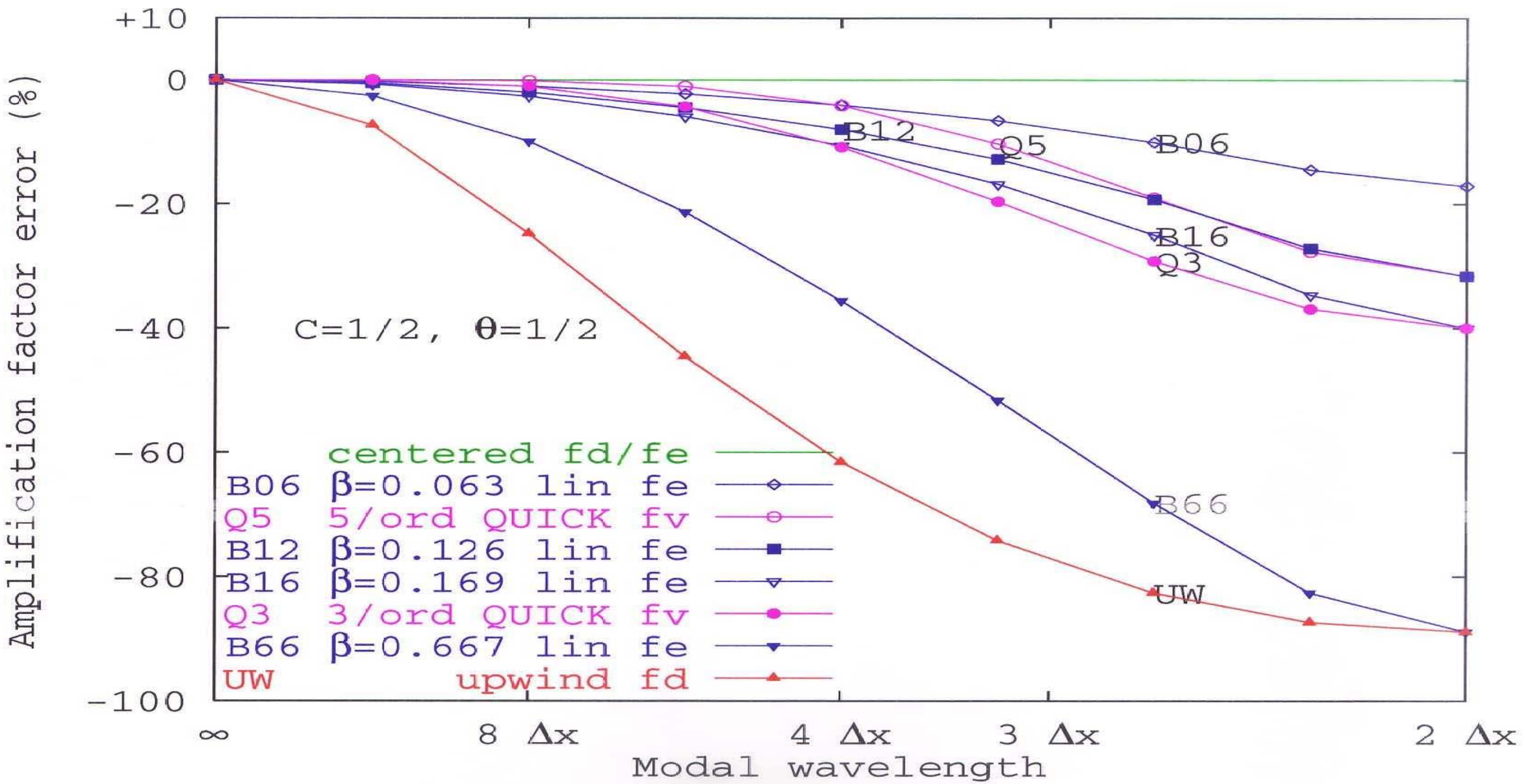
β = 0, γ = -0.5, θ = 0.5

β = 1 = γ, θ = 0



STn.7 Artificial Diffusion Error Spectra

Amplification factor |G| departure from unity



STn.8 GWS^h (*m*D*E*) + θTS, Newton Template *for all n*

Scalar (heat/mass) transport on *n*

D*E*:

$$\mathrm{L}(q) = \frac{\partial q}{\partial t} + u_j \frac{\partial q}{\partial x_j} - \frac{1}{\mathrm{Pa}} \frac{\partial}{\partial x_j}\left[\left(1 + \mathrm{Re}^t\right)\frac{\partial q}{\partial x_j}\right] - s = 0$$

*m*D*E*:

$$\mathrm{L}^m(q) = \mathrm{L}(q) - \frac{\Delta t}{2}\frac{\partial}{\partial x_j}\left[\alpha u_j \frac{\partial q}{\partial t} + \beta u_j u_k \frac{\partial q}{\partial x_k}\right] - \frac{\Delta t^2}{6}\frac{\partial}{\partial x_j}\left[\gamma u_j u_k \frac{\partial^2 q}{\partial x_k \partial t}\right] + \cdots = 0$$

Template pseudo-code additions for STn.2

$$\{\mathrm{WS}\}_e = (\mathrm{const})(\mathrm{avg})_e \{\mathrm{dist}\}_e (\mathrm{metric})[\mathrm{Matrix}]_e \{Q \; or \; \mathrm{data}\}_e$$

$$[m\mathrm{JAC}]_e = [\mathrm{JAC}]_e + (\alpha, \Delta t/2)(\;)\{\mathrm{U}J\}(0)[\mathrm{M}30J0][\;]$$
$$+ (\gamma, \Delta t^2/6)(\;)\{\mathrm{U}J, \mathrm{U}K\}(-1)[\mathrm{M}400JK][\;]$$
$$+ (\beta, \Delta t/2, \theta\Delta t)(\;)\{\mathrm{U}J, \mathrm{U}K\}(-1)[\mathrm{M}400JK][\;]$$

$$\{m\mathrm{RES}\}_e = \{\mathrm{RES}\}_e + \text{added terms } [m\mathrm{JAC}]_e \{Q\}_e$$

STn.9 The "Rotating Cone," n = 2 Mass Transport

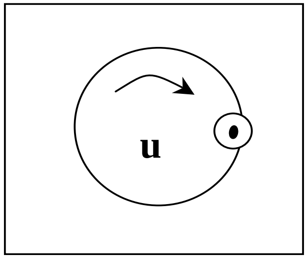
IC & exact solution

$$\text{D}M: \quad \mathrm{L}(q) = q_t + \mathbf{u}\cdot\nabla q = 0$$

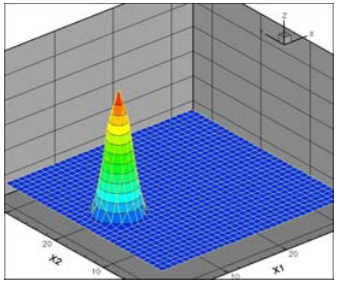
$$\mathbf{u} = r\omega\hat{\mathbf{e}}_\theta$$

$$\text{on } \partial\Omega_{in}: \quad q(\mathbf{x}_b) = q_b \equiv 0$$

$$at\ t_0: \quad q(\mathbf{x}, t_0) = q_0(\mathbf{x}) \Rightarrow \text{"gaussian hill"}$$



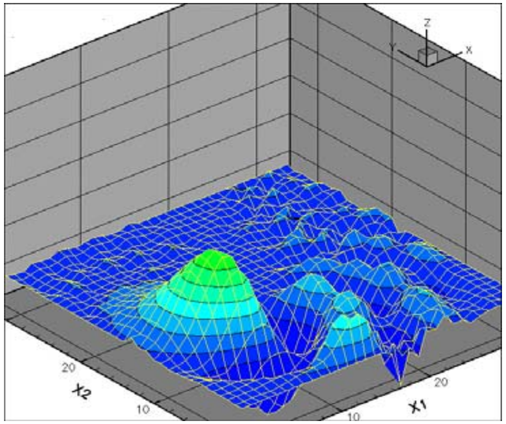
top view



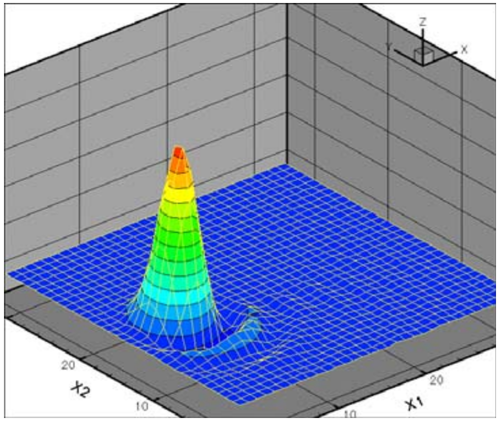
perspective

Select WS ^{h} + θTS solutions, $\overline{\text{C}}$ = 0.5 = θ, one revolution

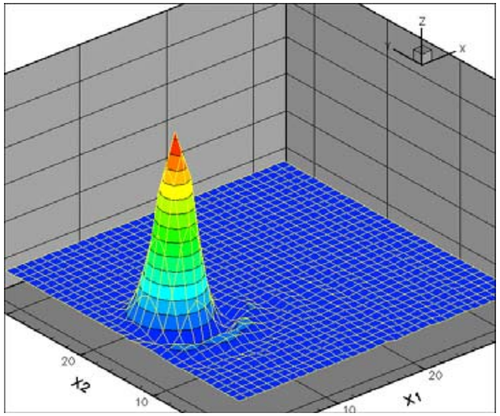
Crank-Nicolson FD



GWS^h k = 1 FE



TWS^h, k = 1 FE
α = 0 = β, γ = -0.5



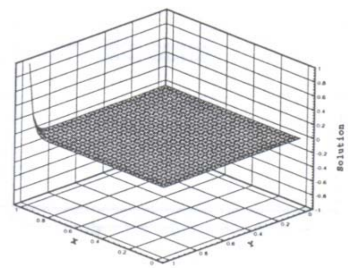
STn.10 The n = 2 Steady Peclet Problem

$$\text{D}E: \; \mathcal{L}(\Theta) = \mathbf{u} \cdot \nabla\Theta - \frac{1}{\text{Pe}} \nabla^2 \Theta = 0$$

$$\text{BCs}: \Theta(x_b) = 0, \quad \Theta(1,1) = 1$$

$$\text{data}: \mathbf{u} = \hat{\mathbf{i}} + \hat{\mathbf{j}}$$

TWS^h solution, M = 30 × 30



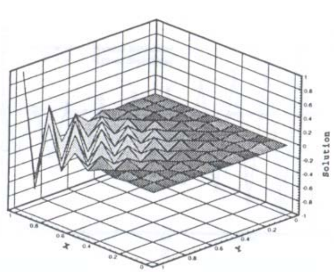
optimal TWS^h:

$$\beta\Delta t / 2 \Rightarrow \text{Pe}\, h^2 / 12$$

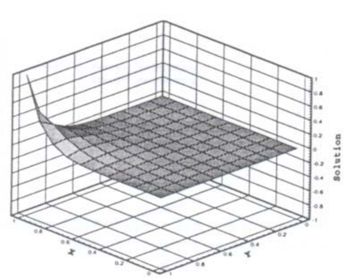
$$\text{error estimate } (k=1): \quad \left\| e^h \right\|_E < C h^4 \left\| \text{data} \right\|^2_{L2}$$

GWS^h, optimal TWS^h solutions, k = 1, Pe = 200

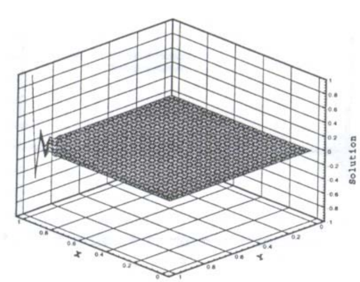
GWS^h, M = 10 × 10



TWS^h, M = 10 × 10



GWS^h, M = 30 × 30



TWS^h convergence, Pe = 10

M	$\left\|Q\right\|_E$ x10^{-5}	$\left\|\Delta Q\right\|_E$ x10^{-5}	Slope
8x8	0.468156		
16x16	0.448714	0.01944	
32x32	0.447985	0.00073	4.74
64x64	0.447945	0.00004	4.19

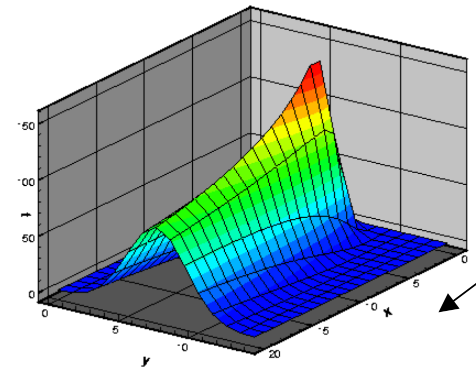
STn.11 The Gaussian Plume, n = 2, 3 Mass Transport

$$\mathrm{D}M : \mathrm{L}(q) = \mathbf{u}\cdot\nabla q - \mathrm{Pa}^{-1}\nabla\cdot(1+\mathrm{Pa}^{t})\nabla q - s = 0$$

$$\mathrm{BCs}: \quad q_{in} = 0,\ \hat{\mathbf{n}}\cdot\nabla q_{out} = 0$$

$$\mathrm{data}: \quad \mathbf{u} = \mathbf{i},\ \mathrm{Pa} \le 100,\ s(\mathbf{x}) = \text{given}$$

$\mathrm{GWS}^h,\ n = 2,\ \mathrm{Pa} = 10,\ \mathrm{Pa}^t = 0\hat{\mathbf{i}} + \hat{\mathbf{j}} - 1$



GWS^h DOF distributions, n = 2

FE $k = 1$

																1	1	2	2	3
						-1				1	1	2	3	5	5	6	8	9	9	10
							4	6	9	12	14	16	18	20	21	22	24	25	25	26
			2	12	21	28	35	38	41	44	45	46	47	48	48	48	49	49	49	49
	0	8	50	93	100	97	96	93	90	88	86	83	81	79	77	75	74	72	71	69
	0	16	92	159	156	142	132	123	116	110	105	100	97	94	90	87	85	82	80	78
U →	0	25	98	162	166	145	137	129	121	115	109	105	100	97	93	90	88	85	83	81
	-2	10	94	169	164	148	138	129	122	116	111	106	101	98	95	91	89	86	83	81
	-1	4	50	97	103	101	98	95	93	90	88	86	83	81	80	77	76	74	73	71
			2	10	19	26	31	35	38	41	43	44	45	46	47	47	48	48	48	48
				-2	-2	-1	1	3	6	9	11	14	15	17	19	20	22	23	24	25
											1	2	2	4	5	5	7	8	8	9
																	1	1	2	2

Gaussian

1
3
10
26
48
71
81

81
71
48
26
10
3
1

source region

FE $k = 2$

STn.12 Mass Transport, FEMLAB Pellet Problem

Conservation principles, fluidized bed creeping flow

flow field

$$\mathrm{D}M : \nabla \cdot \mathbf{u} = 0$$

$$\mathrm{DP} : (\mathbf{u} \cdot \nabla)\mathbf{u} + \frac{1}{\rho_0}\nabla p - \frac{1}{\mathrm{Re}}\nabla^2 \mathbf{u} = 0$$

$$\mathrm{D}M_c : \mathbf{u} \cdot \nabla c - \frac{1}{\mathrm{Re\,Sc}}\nabla^2 c = 0$$

catalyst

$$\mathrm{D}M_c : \quad \frac{1}{\mathrm{Re\,Sc}}\nabla^2 c + kc^2 = 0$$

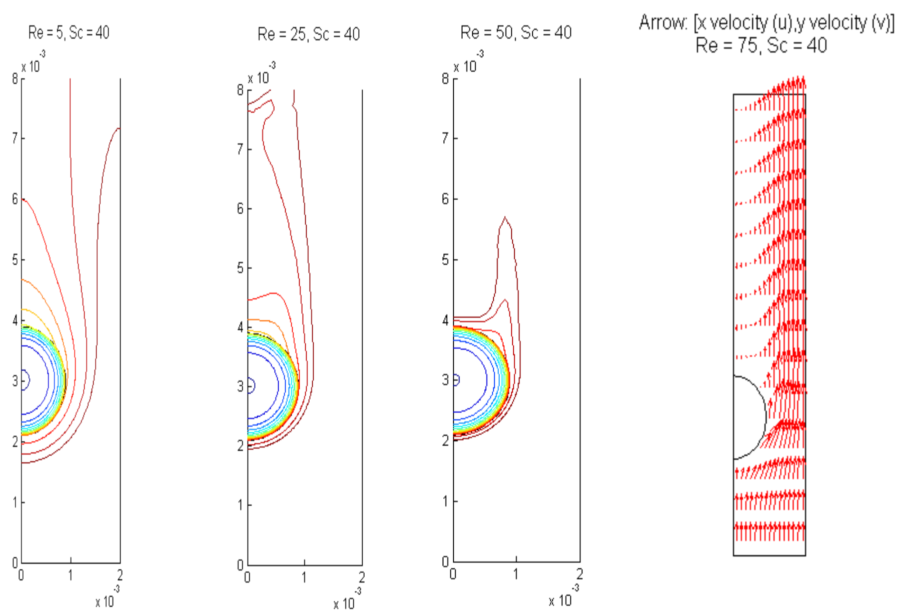
non-D groups

$$\mathrm{Re} = \mathrm{UR} / \nu$$

$$\mathrm{Sc} = \nu / \mathrm{D}$$

mass fraction, velocity contours

Re = 5 | Re = 25 | Re = 50 | Re = 75



STn.13 Summary, Unsteady n – D Scalar Transport

Essential ingredients of GWS^h $(m\mathrm{D}E) \Rightarrow \mathrm{TWS}^h + \theta\mathrm{TS} = \{0\}$

approximation : $q(\mathbf{x},t) \approx q^N(\mathbf{x},t) \equiv q^h(\mathbf{x},t) = \cup_e q_e(\mathbf{x},t)$

FE basis : $q_e(\mathbf{x},t) = \{N_k(\zeta,\eta)\}^T \{Q(t)\}_e$

error extremization : $\mathrm{GWS}^N = \int_\Omega \Psi_\beta(\mathbf{x}) \mathrm{L}^m(q^N)\,d\tau \equiv \{0\} \Rightarrow \mathrm{GWS}^h$

matrix statement : $\mathrm{GWS}^h + \theta\mathrm{TS} \Rightarrow [m\mathrm{JAC}]\{\Delta Q\} = -\Delta t\{m\mathrm{RES}\}$

$[m\mathrm{JAC}] = \mathrm{S}_e([m\mathrm{JAC}]_e), \quad \{m\mathrm{RES}\} = \mathrm{S}_e(\{m\mathrm{RES}\}_e)$

asymptotic convergence : $\left\| e^h(t) \right\|_E \leq C h_e^{f(k,\mathrm{Pe},\beta)} \left\| \mathrm{data} \right\|_{\mathrm{L}2}^2 + C_t \Delta t^{f(\theta)} \left\| q_0 \right\|_E$

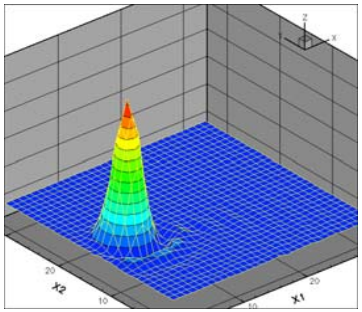
error spectra : U_ω & $G \Rightarrow f(\omega, k, h, \Delta t, \theta, \alpha, \beta, \gamma)$

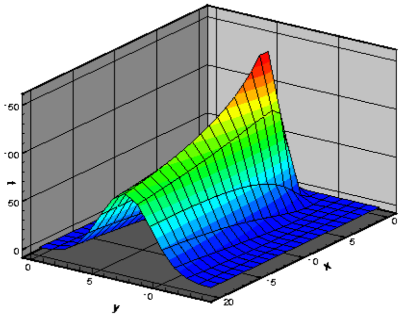
Template pseudo-code converts theory ⇒ practice

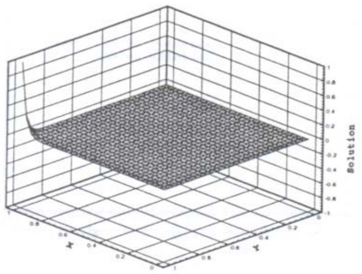
$\mathrm{GWS}^h(m\mathrm{D}E) + \theta\mathrm{TS} \Rightarrow \mathrm{S}_e\{\mathrm{WS}\}_e \equiv \{0\}$

$\{\mathrm{WS}\}_e \equiv (\mathrm{const})(\mathrm{avg})_e\{\mathrm{dist}\}_e(\mathrm{metric})[\mathrm{Matrix}]_e\{Q \textit{ or } \mathrm{data}\}_e$

$[\mathrm{JAC}]_e \equiv \partial\{\mathrm{RES}\}_e / \partial\{Q\}_e$







STn.8A CFD Algorithm Error Spectra