

Direct Evaluation of

3D Hypersingular Galerkin Integrals

L. J. Gray

Oak Ridge National Laboratory

Outline

- **Direct Evaluation:**
 - definition as limit to the boundary – finite integrals
 - polar coordinates: $\rho d\rho$ reduces singularity and ρ integrated analytically
 - *explicit* identification and cancellation of divergences for coincident & edge-adjacent integrals
- **Surface gradient evaluation**

Hypersingular Integral: Laplace

Collocation:

$$\int_{\Sigma} \phi(Q) \frac{\partial^2 G}{\partial N \partial \mathbf{n}}(P_0, Q) dQ$$

Galerkin:

$$\int_{\Sigma} \psi_k(P) \int_{\Sigma} \phi(Q) \frac{\partial^2 G}{\partial N \partial \mathbf{n}}(P, Q) dQ dP$$

$$\frac{\partial^2 G}{\partial N \partial \mathbf{n}}(P, Q) = \frac{1}{4\pi} \left(\frac{\mathbf{n} \cdot \mathbf{N}}{r^3} - 3 \frac{(\mathbf{n} \cdot \mathbf{R})(\mathbf{N} \cdot \mathbf{R})}{r^5} \right)$$

$\mathbf{R} = Q - P \quad r = \|\mathbf{R}\|$

$r = 0$

Galerkin: Divergent Integrals

Interpolation: $\phi(Q) = \sum_j \phi(Q_j) \psi_j(Q)$

$$\phi(P_j) \int_{E_P} \psi_k(P) \int_{E_Q} \psi_j(Q) \frac{\partial^2 G}{\partial N \partial n}(P, Q) dQ dP$$

An individual integral is **divergent** if:

- $E_P = E_Q$
- E_P and E_Q share an edge

Root cause is same as C^1 , must integrate over complete neighborhood of the singularity.

Galerkin Evaluation in 3D

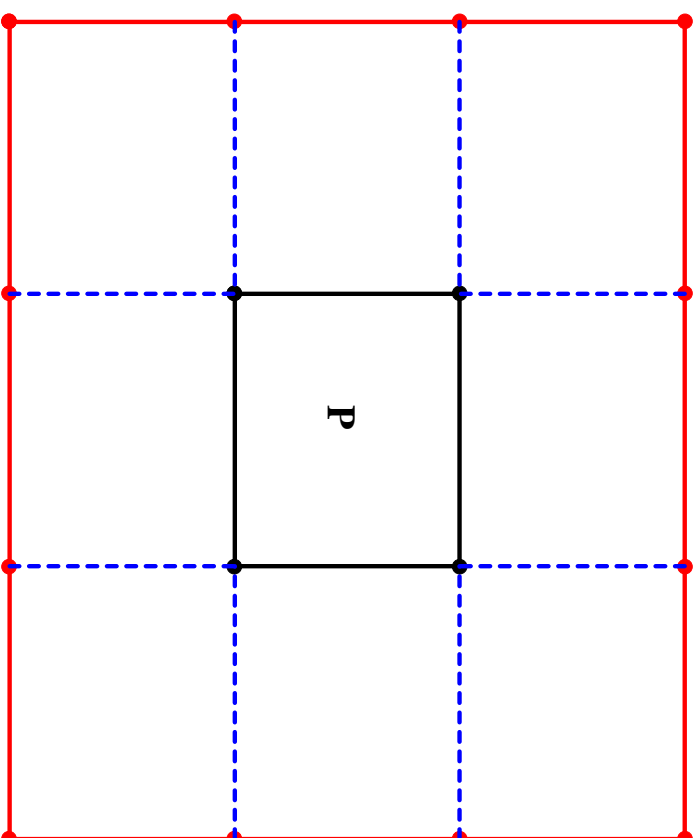
Stokes' Theorem: (Li & Mear, Frangi & Novati, Bonnet, Lutz)

- finite integrals
- contour integral
- 'smearing' of local contributions, generality(?) (e.g., FGM Green's functions)

Hadamard Finite Part: (Salvadori & Carini)

- analytic integration (for inner integral)
- artificially removes singularity
- complicated, generality(?)

Stokes Contour



Limit Direct

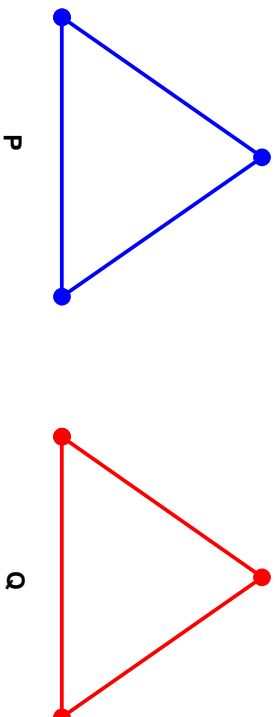
Goals:

- Materialize divergent terms
- Prove cancellation
- Generally applicable algorithm

Method:

- **Boundary Limit:** $P \rightarrow P + \epsilon N$
- Change variables, swap integrations, analytic ρ integration
- Cancellation via complete integration

Parameter Spaces



Equilateral triangle: $dP \rightarrow d\xi d\eta$ $dQ \rightarrow d\xi^* d\eta^*$

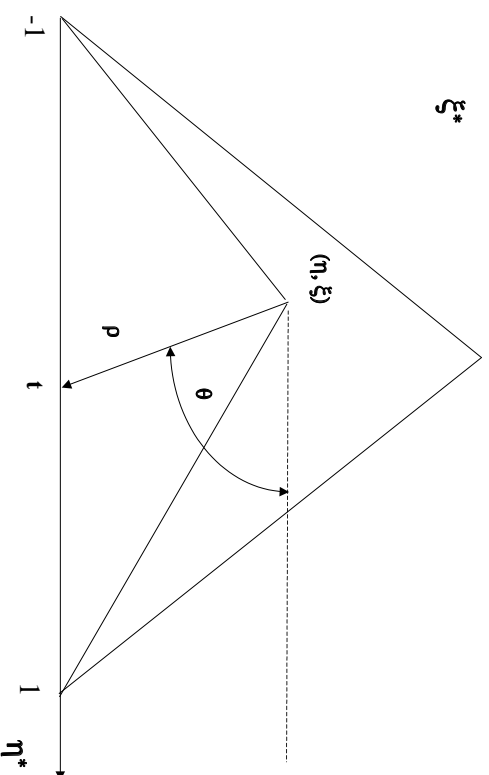
$$-1 \leq \eta \leq 1 \quad 0 \leq \xi \leq \sqrt{3}(1 - |\eta|)$$

Linear Element: $\psi_1(\eta, \xi) = (1 - \eta - \xi/\sqrt{3})/2$

$$\psi_2(\eta, \xi) = (1 + \eta - \xi/\sqrt{3})/2$$

$$\psi_3(\eta, \xi) = \xi/\sqrt{3}$$

Coincident: First Integration

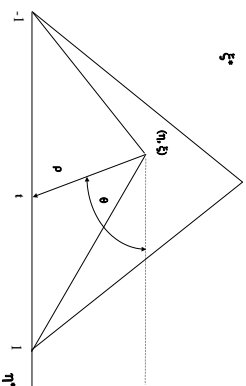


$$r^2 = a^2 \rho^2 + \epsilon^2$$

$$\int_{-1}^1 d\eta \int_0^{\sqrt{3}(1-|\eta|)} d\xi \int_{\theta_1(\eta,\xi)}^{\theta_2(\eta,\xi)} \frac{\rho_L^2}{(\epsilon^2 + a^2 \rho_L^2)^{3/2}} d\theta$$

$$\rho_L \rightarrow 0 \text{ for } \xi \rightarrow 0$$

Coincident: continued



$$\int_{-1}^1 d\eta \int_0^{\sqrt{3}(1-|\eta|)} d\xi \int_{\theta_1}^{\theta_2} \frac{\rho_L^2}{(\epsilon^2 + a^2 \rho_L^2)^{3/2}} d\theta$$

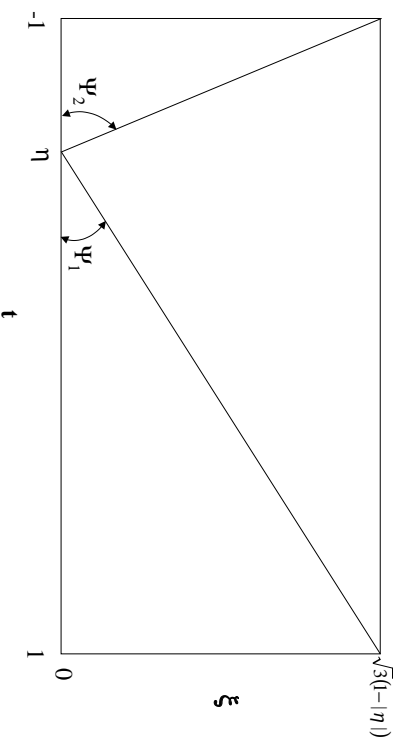
Change of Variables: $\theta = -\frac{\pi}{2} + \tan^{-1}\left(\frac{t-\eta}{\xi}\right) \quad -1 \leq t \leq 1$

$$\int_{-1}^1 d\eta \int_{-1}^1 dt \int_0^{\sqrt{3}(1-|\eta|)} \dots \frac{d\xi}{[\epsilon^2 + a^2(\xi^2 + (t-\eta)^2)]^{3/2}}$$

Coincident: Second Integration

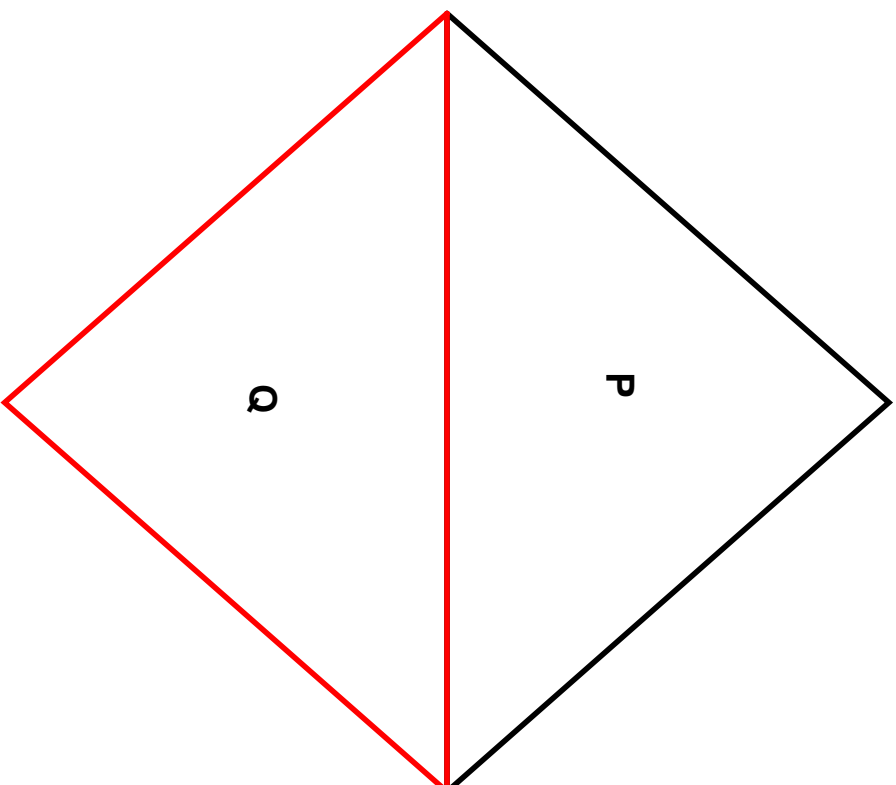
Denominator suggests another polar transformation for (t, ξ)

$$t - \eta = \Lambda \cos(\Psi) \quad \xi = \Lambda \sin(\Psi)$$



$$\int \frac{\Lambda^2}{(\epsilon^2 + a^2 \Lambda^2)^{3/2}} d\Lambda \rightarrow \log(\epsilon)$$

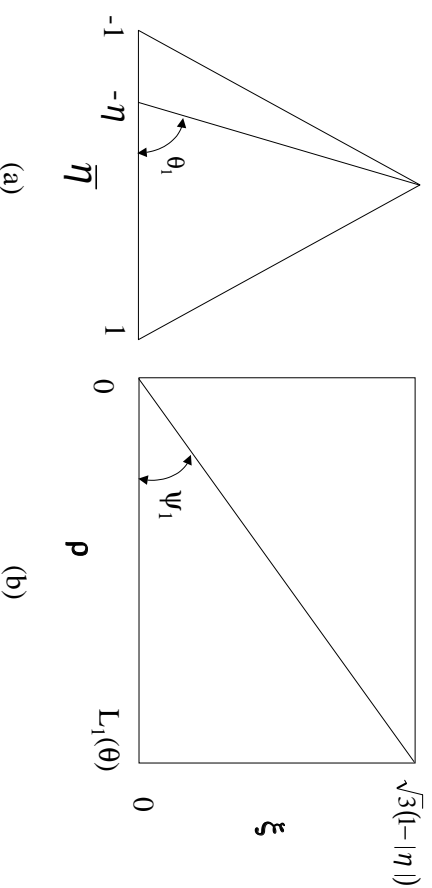
Adjacent Edge



Singularity at:

$$\xi = \xi^* = 0$$

$$\eta = -\eta^*$$



1. Polar coordinates (ρ, θ) centered at $(-\eta, 0)$ replacing (η^*, ξ^*)
2. θ_1 only a function of $\eta \Rightarrow$ interchange ξ and θ
3. Polar coordinates (Λ, Ψ) replacing (ρ, ξ) ; (η, θ, Ψ) numerically
4. Jacobian $= \Lambda^2 \cos(\Psi)$; $r^2 = \epsilon^2 + a_1\epsilon\Lambda + a_2\Lambda^2$

Comments

- Analytic integration is always wrt distance from the singularity
- Equilateral parameter space for convenience – coincident integration
- Proving cancellation of the $\log(\epsilon)$ terms takes some work – remaining dimensions must be integrated
- **Adjacent Edge:** limit direction not necessarily normal
- Most of the grunge work handled by symbolic computation

Limit vs. Stokes

Simplicity is in the eye of the beholder

- Gradient evaluation
- FGM Green's Functions
- Conditioning (?): nonlinear boundary conditions (electrochemistry, crack friction, etc.)

Gradient applications:

- Moving boundary problems: wave motion, electromigration, crystallization, etc.
- Nonlinear: Contact analysis, Shape optimization

Galerkin Gradient I

$$\int_{\Sigma} \hat{\psi}_k(P) \frac{\partial \phi}{\partial \mathbf{E}_k}(P) dP = \lim_{P_I \rightarrow P} \int_{\Sigma} \hat{\psi}_k(P)$$

$$\int_{\Sigma} \left[\frac{\partial G}{\partial \mathbf{E}_k}(P_I, Q) \frac{\partial \phi}{\partial \mathbf{n}}(Q) - \phi(Q) \frac{\partial^2 G}{\partial \mathbf{E}_k \partial \mathbf{n}}(P_I, Q) \right] dQ dP$$

$$A \left[\frac{\partial \phi(P_j)}{\partial \mathbf{E}_k} \right] = b$$

A is sparse, symmetric positive definite
 b is an **expensive** computation

Galerkin Gradient II

Exterior Limit Equation:

$$0 = \lim_{P_E \rightarrow P} \int_{\Sigma} \hat{\psi}_k \int_{\Sigma} \left[\frac{\partial G}{\partial \mathbf{E}_k} (P_E, Q) \frac{\partial \phi}{\partial \mathbf{n}} - \phi \frac{\partial^2 G}{\partial \mathbf{E}_k \partial \mathbf{n}} (P_E, Q) \right] dQ dP$$

$$\frac{\partial \phi(P)}{\partial \mathbf{E}_k} = \left\{ \lim_{P_I \rightarrow P} - \lim_{P_E \rightarrow P} \right\} \int_{\Sigma} \hat{\psi}_k \int_{\Sigma} \left[\frac{\partial G}{\partial \mathbf{E}_k} \frac{\partial \phi}{\partial \mathbf{n}} - \phi \frac{\partial^2 G}{\partial \mathbf{E}_k \partial \mathbf{n}} \right] dQ dP$$

1. *Only terms that are discontinuous crossing boundary: coincident, hypersingular adjacent edge (low order terms from shape functions)*
2. Requires a limit definition
3. Collocate limit difference?

Penny-shaped crack

Disk:

$$x^2 + y^2 \leq R_0^2 \quad z = 0$$

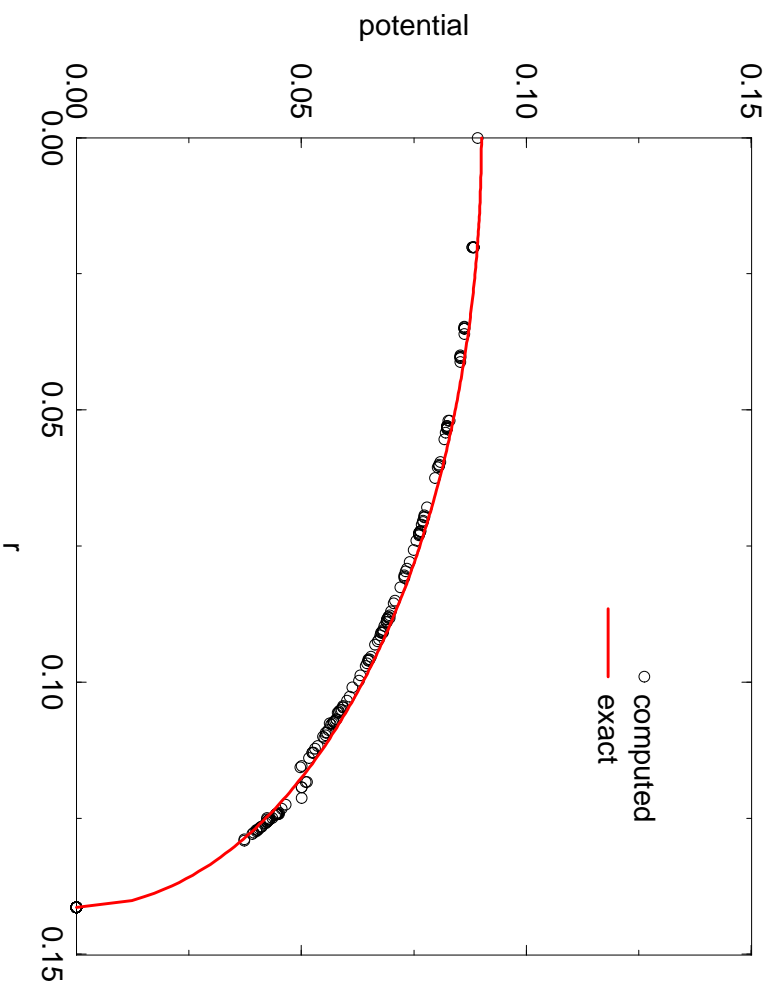
Boundary condition:

$$\left[\frac{\partial \phi}{\partial \mathbf{n}} \right] = \frac{\partial \phi}{\partial \mathbf{n}}(P^+) + \frac{\partial \phi}{\partial \mathbf{n}}(P^-) = 1$$

Solution:

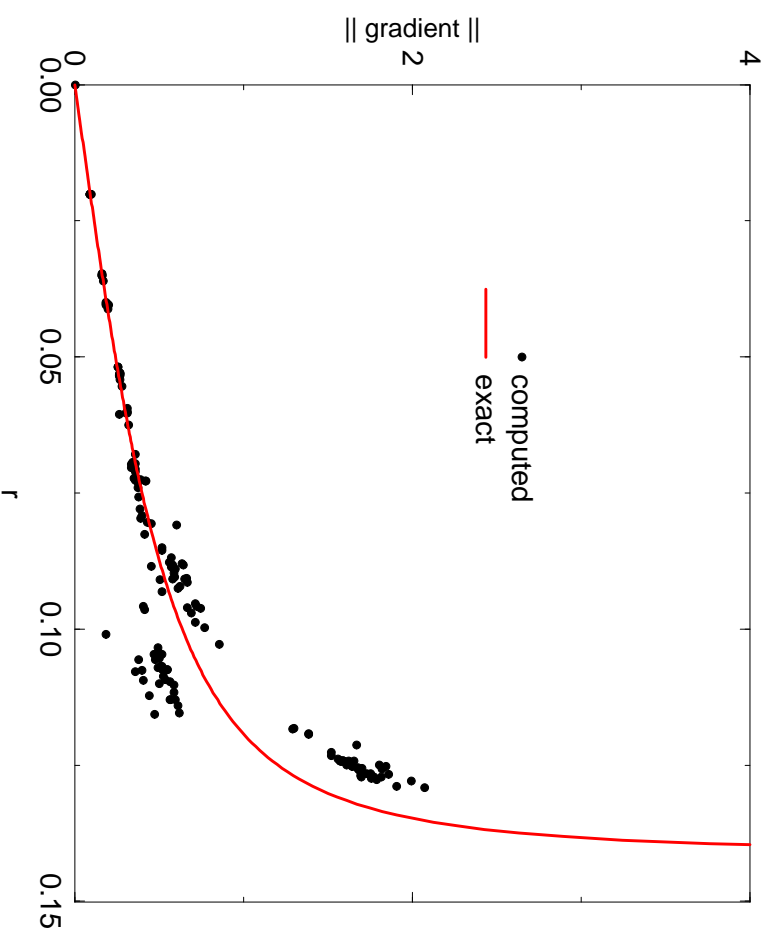
$$[\phi] = \phi(P^+) - \phi(P^-) = \frac{2R_0}{\pi} \sqrt{1 - \frac{r^2}{R_0^2}}$$

Penny-shaped crack



The solution for $[\phi]$ for the pressurized penny shaped crack.

Penny-shaped crack



Current Work

- Higher order elements: linear analysis plus remainders

$$(a_4\rho^4 + a_3\rho^3 + a_2\rho^2 + \epsilon^2)^{-1/2} = (a_2\rho^2 + \epsilon^2)^{-1/2} + \text{Rem}$$

- Green's functions: elasticity (Phan), FGM (Sutradhar), anisotropic elasticity
- Conditioning
- Numerical integrations

Anisotropic Elasticity

$$U_{kj}(Q, P) = \frac{1}{8\pi^2 r} \tilde{U}_{kj}(\theta, \psi)$$

$$U_{kj,lm}(Q, P) = \frac{1}{8\pi^2} \left[\left(\frac{\delta_{lm}}{r^3} - 3 \frac{(q_l - p_l)(q_m - p_m)}{r^5} \right) \tilde{U}_{kj}(\theta(\epsilon), \psi(\epsilon)) + \dots \right]$$

Taylor expansion for \tilde{U}_{kj}

Summary

- **Direct**, **general**, simple, 3D singular integration algorithms
- Limit definition essential for **fast** surface gradient method

Collaborators

- Julia Glaeser (summer undergrad)
- Anh-Vu Phan (ORNL)
- Ted Kaplan (ORNL)