Fitting boundary-value problems to data

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Data from following physical inverse problems:

- Acoustic imaging. Helmholtz Eqn. in plane.
- Electrical imaging. Diffusion Eqn. in disk.
- Detect abyssal ocean currents. Advection-diffusion Eqn. in rectangular window.
- Geothermal reservoir. Two phase flow in half-space.

- What kind of information does the data contain?
- Estimate physical parameters.

Sample-based Bayesian inference with expensive likelihood calculations:

- Approximate likelihood, use coupling-separation to control approx.
- Get serial depth via parallel implementation.
\[
U(x, t) = u(x)e^{-i\omega t} \quad \text{with} \quad u(x) = u_i(x) + u_s(x)
\]

\[
\nabla^2 u + k^2 u = 0 \quad \text{in} \quad \Omega \subseteq \mathbb{R}^2
\]

\[
\frac{\partial u}{\partial n} = 0 \quad \text{in} \quad \partial\Omega \quad \text{and} \quad \lim_{r \to \infty} r \left( \frac{\partial u_s}{\partial r} - ik u_s \right) = 0
\]

Estimate polygonal inclusion - i.e. $\partial\Omega$ - given $u_i$ and noisy measurements of $u_s(x_k)$ at $x_k \in \Omega, k = 1, 2\ldots K$

Boundary element method for $u_s(\partial\Omega)$
Apparatus; $\sigma_{MAP}$ Gauss-Newton optimization; $\sigma_{PM}$ and variance.

$$\nabla \cdot (\sigma \nabla) u = 0 \quad \text{in } \Omega \subseteq \mathbb{R}^2, \quad \sigma : \Omega \rightarrow \mathbb{R}^+$$

$$\frac{\partial u}{\partial n} = J_{\partial \Omega} \quad \text{in } \partial \Omega$$

Estimate $\sigma(x)$, $x \in \Omega$ given measurements of $(v, J_{\partial \Omega})$

$v = u(\sigma; J_{\partial \Omega}) + \text{agn.}$

$$\pi(\sigma \mid V) \sim \exp \left\{ - \left( \frac{1}{2} (V - U(\sigma))^T C^{-1}_n (V - U(\sigma)) \right) \right\} \pi_{pr}(\sigma)$$

Complete-electrode model/FEM for $U(\sigma)$
Observation model (2D) Data: $C_D^{(t)}$, Parameters: $\Psi$

$t = \text{salinity, oxygen, Si, potential temperature}$

2D advection diffusion on an isopycnal $\Gamma(x, y, z) = \Gamma_0$

$$uC_x^{(t)} + vC_y^{(t)} - (k_x^{(x)}C_x^{(t)})_x - (k_y^{(y)}C_y^{(t)})_y = -\lambda^{(t)}C^{(t)}$$

Dynamics:

$$\beta v = fw_z \quad u = \int_x^{x_E} (-v_y - \beta v/f)dx'$$

using 3D mass conservation $\nabla \cdot u = 0$ with boundary condition $u(x_{East}) = 0$.

$$\Psi = (v, k_x^{(x)}, k_y^{(y)}, C_{\partial\Omega})$$

Measurement:

$$C_D^{(t)}(x, y, z) \sim N(C^{(t)}(x, y, z), \sigma_t^2)$$

Posterior:

$$P(\Psi|C_D) \propto P(C_D|\Psi)P(\Psi)$$

Multigrid method for each $C_t^{(t)}$
Radial symmetric model, homogeneous constant thickness layer (200m) infinite extent. One rock type, estimate

Parameters: $\Psi = (\phi, k, S_{lr}, S_{vr}, p_0, S_{v0})$

$\phi$ porosity, $k$ permeability in radial direction $S_{lr}, S_{vr}$ liquid and vapour residual saturations, $p_0$ initial pressure and $S_{v0}$ initial vapour saturation fields

Data: $D = (h_{D,f}^{(t_j)}, p_D^{(t_j)}, q_{D,m}^{(t_i)}, t_i), i = 1, 2..I, j = 1, 2..J$

Drive: $q_{D,m}^{(t_i)}$ production rate, $t(.)$ time, days.

Response: $h_{D,f}^{(t_j)}$ flowing enthalpy, $p_D^{(t_j)}$ wellhead pressure

Observation model:
Forward model: $\Psi, q_{D,m} \rightarrow h_f, p$.
Measurement model: $h_{D,f}, p_D = h_f, p + \text{agn}$.

Solve via finite element analysis:

Sample based inference  
Summarize $P(\Psi|D) \propto P_D(D|\Psi)P_\Psi(\Psi)$ using samples $\psi_i \sim P, \quad i = 1...N$: 
Correlated $\psi_i \sim P, \quad i = 1...N$ from MCMC 

MCMC 
Fix an operator $\psi' = \Psi(\psi, u)$ and for $i = 0, 1, 2..., v_i \sim U(0, 1)$ and $u_i \sim a(u_i)$.  
**function** $\psi_{i+1} = \text{Next}(\psi_i, v_i, u_i, P)$  
  1. set $\psi' = \Psi(\psi, u_i)$ 
  2. compute  

\[
\alpha(\psi'|\psi; P) = \min \left( 1, \frac{P(\psi'|D)a(u'_i)}{P(\psi|D)a(u_i)} \left| \frac{\partial(\psi', u'_i)}{\partial(\psi, u_i)} \right| \right)
\]

  3. if $v_i < \alpha(\psi'|\psi; P)$ set $\psi_{i+1} = \psi'$ else $\psi_{i+1} = \psi$.  

[eg] Fix $s \in (0, 1)$, set $u_i \sim U(1/s, s)$ and $\phi' = (\phi, k, S_{lr}, u_i S_{vr}, p_0, u_i S_{v0})$. 
Then $u'_i = 1/u_i$, Jacobian is 1 and  

\[
\alpha(\psi'|\psi; P) = \min \left( 1, \frac{P(C_D|\psi')P(\psi')}{P(C_D|\psi)P(\psi)} \right)
\]
Approximation-choice strategy: coupling-separation $\tilde{\psi}_0 = \psi_0$

$\psi_{i+1} = \text{Next}(\psi_i, v_i, u_i, P)$  \quad  $\tilde{\psi}_{i+1} = \text{Next}(\tilde{\psi}_i, v_i, u_i, \tilde{P})$

Chains start together, separate $\psi_{i+1} \neq \tilde{\psi}_{i+1}$

$$\min(\alpha_i, \tilde{\alpha}_i) < v_i < \max(\alpha_i, \tilde{\alpha}_i)$$

where $\alpha_i = \alpha(\psi'|\psi; P)$ and $\tilde{\alpha}_i = \alpha(\psi'|\psi; \tilde{P})$.

Samples from $\tilde{\Psi}$-chain identical to “exact” chain up to separation time. $\tilde{\Psi}$-chain need not be Markov. Equilibrium need not exist.

Separation times

$$\tau(\psi_0) = \min\{i > 0; \psi_{i+1} \neq \tilde{\psi}_{i+1} | \Psi_0 = \psi_0\}$$

$$\tau_r = \text{interval between events } \min(\alpha_i, \tilde{\alpha}_i) < v_i < \max(\alpha_i, \tilde{\alpha}_i)$$

$$\tau_r = 1/E(|\alpha_i - \tilde{\alpha}_i|)$$

Estimate $\tau_r$ using short runs of “exact” chain. Choose approximation so that $\tau_r$ exceeds MCMC simulation length.

Acoustic imaging: Likelihood via $O(n^3)$ $n$-boundary element approx. to BVP.

$\Psi$-chain $n = 1024$ - reproduce* experimental data, mixing time 40 updates.

$\tilde{\Psi}$-chain # boundary elements 512 obtain $\tau_r = 1400$ updates.
Parallel implementation:

Biasing correlation between $\Phi_0$ and $\Psi_i$ (burn-in). Serial-depth important.

Strategy. $\Psi_i = \psi$ and fix $n > 0$.

Compute $X_1 = \text{Next}(\psi, \ldots), \ldots, X_n = \text{Next}(\psi, \ldots)$ in parallel.

Let $m = \min\{i = 1, 2, \ldots, n; X_i \neq \psi\}$ (first acceptance).

Set $\Psi_{i+1} = X_1, \ldots, \Psi_{i+m} = X_m$ and throw out $X_{m+1}, \ldots, X_n$.

OpenMosix cluster (about 15 CPUs) for Fushime geothermal data.

Each $P_D(D|\Psi)$—evaluation about 5 seconds. Remote processes via ssh.

Very straightforward implementation.
Further information for geothermal two-phase flow model
\[
\frac{\partial M_m}{\partial t} + \nabla \cdot Q_m = q_m \quad \frac{\partial M_e}{\partial t} + \nabla \cdot Q_e = q_e
\]

\(M_m, M_e\) mass and energy per unit volume, \(Q_m, Q_e\) mass and energy flux per unit area, \(q_m, q_e\) mass and energy injected or withdrawn at wells. Underground geothermal flows:

\[
M_m = \phi(\rho_l S_l + \rho_v S_v) \quad M_e = (1 - \phi) \rho_r c_r T + \phi(\rho_l u_l S_l + \rho_v u_v S_v)
\]

\(S_l + S_v = 1\)

\(\phi\) porosity \(\rho_l, \rho_v\) and \(\rho_r\) liquid, vapour and rock densities \(S_l, S_v\) liquid and vapour saturations. \(u_l, u_v\) and \(c_r\) specific internal energies for liquid and vapour and specific heat of rock respectively. \(T\) temperature.

Two phase Darcy’s Law:

\[
Q_{ml} = -\frac{k k_{rl}}{\mu_l} (\nabla p - \rho_l g) \quad Q_{mv} = -\frac{k k_{rv}}{\mu_v} (\nabla p - \rho_v g)
\]

\[
\begin{pmatrix} k_{rl} \\ k_{rv} \end{pmatrix} = f(S_{lr}, S_{vr}, S_l) \quad Q_m = Q_{ml} + Q_{mv}
\]

\(k\) 3-component permeability \(g\) gravitational acceleration, \(\nabla p\) pressure gradient, \(\mu_l\) and \(\mu_v\) dynamic viscosity of liquid and vapour.

\(k_{rl}\) and \(k_{rv}\) relative permeabilities - interference between phases \(S_{lr}, S_{vr}\) liquid and vapor residual saturation \(S_l\) liquid (vapour) saturation.
\[
\begin{aligned}
&k_{rl} = \tilde{S}^4 \\
&k_{rv} = (1 - \tilde{S}^2)(1 - \tilde{S}^2) \quad \text{(Corey's curve)} \\
&k_{rv} = 1 - k_{rl} \quad \text{(Grant's curve)}
\end{aligned}
\]

where \( \tilde{S} = (S_l - S_r)/(1 - S_{lr} - S_{vr}) \).

Energy flux

\[
Q_e = Q_{ml}h_l + Q_{mv}h_v - K \nabla T
\]

\( h_l, h_v \) liquid and vapour enthalpies \( K \) thermal conductivity in saturated medium.

Thermodynamic relations

\[
\begin{aligned}
&h_l = u_l + \frac{p}{\rho_l}, \quad h_v = u_v + \frac{p}{\rho_v}, \quad h_f = Q_e/Q_m \\
&K = (1 - \phi)K_r + \phi(S_lK_l + S_vK_v)
\end{aligned}
\]

\( K_r, K_l \) and \( K_v \) thermal conductivity of rock, liquid and vapour \( h_f \) is the flowing enthalpy for multiphase flow.

\[
\begin{aligned}
&\frac{\partial}{\partial t}[\phi(\rho_l S_l + \rho_v S_v)] - \nabla \cdot \left[ k_{rl} \left( \nabla p - \rho_l g \right) + \frac{k_{rv}}{v_l} \left( \nabla p - \rho_v g \right) \right] = q_m \\
&\frac{\partial}{\partial t}[\phi(\rho_l c_r T + \phi(\rho_l u_l S_l + \rho_v u_v S_v)] - \nabla \cdot \left[ \frac{h_l k_{rl}}{v_l} \left( \nabla p - \rho_l g \right) + \frac{h_v k_{rv}}{v_v} \left( \nabla p - \rho_v g \right) \right] + \nabla \cdot (K \nabla T) = q_m \\
&\left( \begin{array}{c}
\tilde{k}_{rl} \\
\tilde{k}_{rv}
\end{array} \right) = f(S_{lr}, S_{vr}, S_l)
\end{aligned}
\]
$\rho_l, \rho_v, \mu_l, \mu_v, u_l, u_v, h_l, h_v$ and $h_f$ vary with system temperature ($T$) and pressure ($p$), functions from steam table lookup.